8th photodynamics

INTERNATIONAL MEETING ON PHOTODYNAMICS AND RELATED ASPECTS

Oaxaca, México

October 26-31 2014

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14:30 - 15:00						Excursion				
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Fabrice Dayou
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Ara Apkarian
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Ángel Martín Pendás
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Céline Toubin
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Millard Alexander
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Karen Volke
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Vladimiro Mujica
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George Schatz
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Kaoru Yamanouchi
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Thymine Dimer Repair by Photo-induced Electron Transfer from Proximal Molecules

Jack Simons[1]
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Electronic structure methods were used [1,2] to estimate *differences* in reaction barriers for transfer of an electron from singlet ππ* excited 8-amino-guanine (A) or deprotonated 8-amino-guanine anion (A^-) to a proximal thymine dimer site compared to barriers when ππ* excited 8-oxo-guanine (O) or deprotonated 8-oxo-guanine (O^-) serve as the electron donor. It is predicted that the barrier for photo-excited A should be lower than for photoexcited O, and the barrier for photo-excited A^- should be lower than for photo-excited O^-. Moreover, A, O^-, and A^- are predicted to have ππ* excited states at energies near where O does, which allows them to be excited by photons low enough in energy to avoid exciting or ionizing any of DNA's bases. The origin of the differences in barriers is suggested to be the lower ionization potential of A compared to O and the lower electron detachment energy of A^- compared to O^-. Because O and O^- have been experimentally shown to produce thymine dimer repair, it is proposed that A and A^- are promising repair agents deserving experimental study.

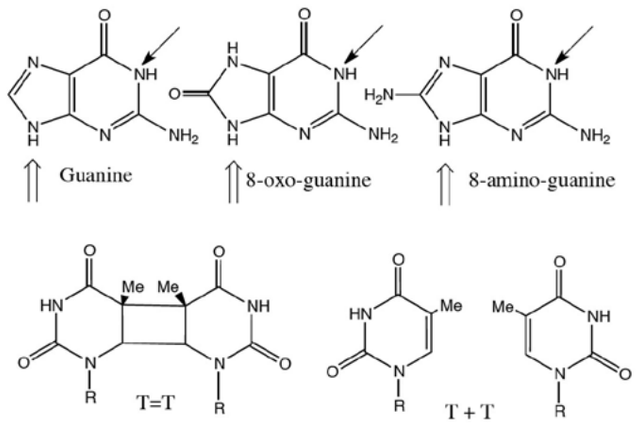

Figure 1. Relevant molecular structures

References

1. I. Sieradzan, M. Marchaj, I. Anusiewicz, P. Skurski, J. Simons, *Prediction of Thymine Dimer Repair by Electron Transfer from Photo-excited 8-amino-guanine or its Deprotonated Anion*, J. Phys. Chem. A (2014) in press.
2. M. Marchaj, I. Sieradzan, I. Anusiewicz, P. Skurski, and J. Simons, *Thymine dimer repair by electron transfer from photo-excited 2',3',5'-tri-O-acetyl-8-oxo-7,8-dihydroguanosine or 2',3',5'-tri-O-acetyl-ribosyluric acid- a theoretical study*, Mol. Phys. 2013, 111, 1580-1588.

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Transient Anion States of Radiosensitizers

M. T. do N. Varella[1], F. Kossoski[1]
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Studies of electron induced damage to biomolecules, in particular DNA and its subunits, have attracted remarkable interest in the last decade [1,2,3]. The high energy photons employed in radiology and radiotherapy generate a large number of secondary species, such as hydroxyl radicals and free electrons, which are largely responsible for DNA damage [4,5]. Low energy (< 30 eV) electrons are the most abundant secondary species and the dissociative processes induced by these electrons are decisive steps in the damage to biomolecules either in the gas or condensed phase [4,5,6]. The key mechanism of the electron induced damage is the formation of a transient anion state (a resonance) whose potential energy surfaces are often dissociative. In contrast, similar electron induced processes can be of help in cancer therapies. Radiosensitizers (e.g. 5-fluorouracil, cisplatin) are chemicals capable of increasing the efficiency of treatments based on UV and ionizing radiation [7]. These sensitizing properties would arise, at least in part, from efficient mechanisms for dissociative electron attachment (DEA). In spite of their importance, the literature on electron interactions with radiosensitizers is relatively scarce, especially on the theory side. In this work, we report on the transient anion states of a well-known class of radiosensitizers, the halouracils, i.e. 5-X-uracils (X=F, Cl, Br, I), and also of 2-thiouracil. Most of the present calculations were carried out employing the parallel version Schwinger Multichannel Method with Pseudopotentials (SMCPP) [8], a well-established computational tool to address electron-molecule collisions. The use of scattering methods is desirable since the bound-state boundary condition is not adequate to metastable states (transient anions). Our calculations point out rich spectra of transient anion states compatible with the available experimental data on electron induced damage to the molecules of present interest. Some of the results have been published recently [9].

References

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Inelastic Collisions of H_2O and O_2 Molecules at Low Temperature by Raman Spectroscopy

José M. Fernández[1], Guzmán Tejeda[1], Elena Moreno[1], Francisco Gámez[1], Estela Carmona-Novillo[2], Marta I. Hernández[2], Salvador Montero[1]
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Raman spectroscopy of supersonic gas jets has been employed along the last ten years [1-5] to study rotationally-inelastic collisions of a number of small molecules at temperatures below 100 K. Number densities and rotational populations can be directly measured along the jet axis from the rotational and/or vibrational Raman spectra. From these primary data, rotational and translational temperatures can be obtained, the latter from conservation of mass, momentum, and enthalpy along the jet. These measurements can be linked to calculations of state-to-state rate coefficients (sts-rates) by means of the kinetic Master Equation, which accounts for the time evolution of the rotational populations. A careful analysis of the Master Equation, which combines experimental and theoretical data, allows one to assess the accuracy of the calculated sts-rates and, in turn, of the potential energy surface (PES).

After an introduction to the experimental technique, we will show our recent measurements in jets involving O_2 and H_2O(gas) molecules diluted in He. Oxygen molecules are cooled down to ~2 K, showing the relaxation among the fine structure triad of the ground rotational state. The rotational populations of H_2O progressively deviate from the Boltzmann distribution, preventing to define a proper rotational “temperature” and affecting the collisional dynamics to a significant extent. Our results will be compared with calculated sts-rates for O_2:He [6], and H_2O:He collisions with three different PES’s [7-9].

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Collisions of Water with Helium: Calculations versus Experiment

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A detailed knowledge of the collisional excitation of water by He is very important for the modeling of water-rich regions in the interstellar medium. Since the pioneering calculations of the H_2O-He potential energy surface (PES) and rotationally inelastic rate coefficients by Green *et al* [1], several improved calculations of PESs have been reported more recently [2-4]. Rate coefficients may be substantially different using one or another PES due to the high sensitivity of the dynamics to their features.

We will report a combined experimental-theoretical study for the determination of the state-to-state rate coefficients of *ortho*- and *para*-H_2O:He inelastic collisions in the 20-120 K thermal range. In the experiment, the H_2O rotational populations along a supersonic jet of a mixture of He and highly diluted H_2O are accurately measured using Raman spectroscopy. On the other hand, rate coefficients are computed by means of close-coupling calculations using the different PESs [2-4]. These calculations are tested against the experiments through a detailed analysis of the kinetic Master equation which combines both experimental and theoretical data. It is found that the rates based on the Hodges[2] and Patkowski[3] PESs agree with experiment within 15%, while the rates by Green[1] are between 25-40% too low.

In this contribution, we will give an analysis of the different H_2O-He PESs and their effects on the rotationally inelastic dynamics. This assessment will be completed by calculations of total integral cross sections in comparison with molecular beam experiments[5]. Finally, a preliminary estimation of water-water rate coefficients (affecting less diluted mixtures) will be reported.

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8th photo dynamics

Photodissociation dynamics studies using the fast imaging PImMS camera

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Keywords: Photodissociation, Imaging mass spectrometry, fast CMOS imaging camera, PImMS

Recent work on the development of a fast imaging camera, known as the Pixel Imaging Mass Spectrometer (or PImMS) camera will be described [1–3]. This camera has been developed in collaboration between the Physics and Chemistry Departments at Oxford University, and the Rutherford Appleton Laboratory, Science and Technology funding Council, UK.

The talk will principally focus on example applications of the PImMS camera to molecular photodissociation [4], including studies of molecular photofragmentation using correlation [5] and three-dimensional imaging techniques. Applications of the PImMS camera to other fields, such as imaging mass spectrometry of surfaces[6], will also be touched on briefly in the presentation. Future potential developments and applications will also be discussed.

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8th photo dynamics

Angular Momentum Polarization in the Photodetachment of Alkali Atoms from Helium Nanodroplets

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The theory of photofragments angular momentum polarization is applied to the photodetachment of an electronically excited alkali atom from a Helium nanocluster (N=200, 1000) [1]. The alignment of the electronic angular momentum of the excited alkali atom produced is calculated quantum mechanically solving the excited states coupled equations with potentials determined by He-DFT. Detailed results will be presented for Na@(^{4}He)$_{200}$, and preliminary results for Na@(^{4}He)$_{1000}$ and Li@(^{4}He)$_{200}$.

Pronounced oscillations as a function of excitation energy are predicted for the case of the alignment parameter, which is proportional to the fluorescence polarization. This is in marked contrast with the absorption cross-section and with the anisotropy parameter of the angular distribution of the ejected atoms, which are smooth functions of energy. These pronounced oscillations should be clearly visible in the fluorescence polarization of the ejected alkali atom.

Preliminary results for Na@(^{4}He)$_{1000}$ indicate that their frequency is dependent on the droplet size, which can be of great practical interest. The effect of nonadiabatic transitions is also shown.

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Molecular modeling of the interaction of halogenated molecules with the ice surface

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The interaction between ice and halogenated species has received much attention in the past few years in the context of atmospheric chemistry and ozone depletion [1].

Chlorine molecules are a major source of Cl radicals. Even if some experimental data (desorption energy, photodissociation cross sections…) are available, their interaction and photodissociation at the ice surface are not fully characterized from a theoretical point of view.

The work we present here concerns first the construction of an *ab initio* derived [2] analytical potential for the Cl_2…H_2O dimer and second the molecular dynamics (MD) simulations of a Cl_2 molecule and a CH_3Cl molecule adsorbed at the surface of ice. The adsorption energy for Cl_2 / ice system, derived from the simulations is in better agreement with experimental data [3,4] than previous estimate based on quantum mechanical calculations on a small cluster [5].

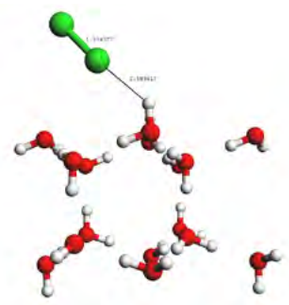

Figure 1. Side view of the Cl_2 molecule adsorbed on ice

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Towards transdermal drug delivery using thermocavitation

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Cavitation is a well-known phenomenon that has found applications in many research fields, including biomedicine. Acoustic cavitation is a well sought approach for controlled tissue damage including thrombolysis, lipoplasty, wound healing, fracture healing, and sonoporation [1]. In the present work, the potential of the relatively unexplored method of thermocavitation, i.e., cavitation induced by continuous wave (CW) low power lasers in absorbing solutions [2] is explored as an alternative method to enhance the permeation of the stratum corneum (SC) and facilitate transdermal drug delivery (TDD). The collapse of cavitation bubbles microscopically disrupt the lipid bilayers of the SC to allow the permeation of drugs [3]. In this work, the damage induced on softer materials, such as agar gels and *ex-vivo* porcine skin itself is studied as a preamble to studies on thermocavitation for tissue ablation. Further approaches on permeation of SC are also discussed such as water jets generated by thermocavitation in a single water droplet or in microfluidic channels. This last approach seems suitable for practical needless drug delivery.

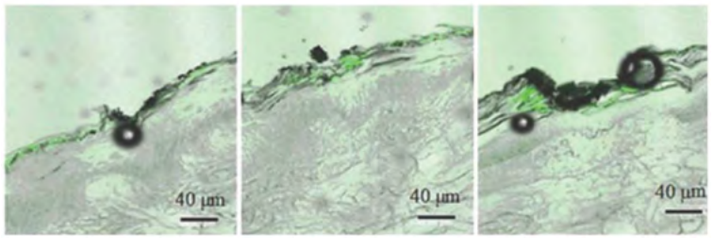

Figure 1. Laser scanning confocal images for pork skin sections where the FITC dextran solution (shown in green) was topically applied for 2.5 h. SC is clearly broken by thermocavitation.

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Light-matter and phonon-exciton interactions in purple bacteria LHII

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We have been investigating light absorption and exciton dynamics in the structurally well-characterized light-harvesting apparatus of purple bacteria. In particular, we have investigated the strength of conclusions drawn about exciton locality and depolarization based on femtosecond laser experiments. As part of this work we have used molecular dynamics and density functional theory to parameterize physically realistic model Hamiltonians of the system, allowing us to investigate exciton transport and decoherence of excitonic states. Here our recent progress in understanding the formation of the initial excited state and its subsequent dynamics will be discussed, as will the light-matter interaction in the different regimes of continuous-wave laser radiation, femtosecond pulses and low-intensity incoherent light.

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Solvent Effect on the Stokes Shift and on the Non- Fluorescent Decay of Daidzein

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In this work we present a theoretical investigation of the role of the solvent in the large Stokes shift experimentally observed in the daidzein molecular system in water. The non-fluorescent decay mechanism in polar aprotic solvent is also addressed. The solvent effect in the ground and in the low-lying excited electronic states is taken into account by using the Sequential-QM/MM methodology. Excited state properties like equilibrium geometries and transition energies were studied by using multiconfigurational calculations, CASSCF and CASPT2. The excited electronic state responsible for the fluorescence spectrum in water was identified and the large Stoke shift seems to be the result of the large interaction of the system in this electronic state with the solvent. In addition, spin-orbit coupling calculations, between the singlet and triplet electronic states of daidzein in acetonitrile, indicate favorable conditions for intersystem crossing, in agreement with the experimental result of non-fluorescence observation.

This work has been partially supported by CNPq, CAPES and FAPESP.

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Energy Funneling and Excited State Dynamics in Conjugated Dendrimers

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Light-harvesting and intramolecular energy funneling are fundamental processes in natural photosynthetic systems, biosensors, and a large variety of organic photovoltaic devices. Dendrimeric macromolecules are artificial light-harvesting molecules possessing unique architectures that allow the efficient energy funneling through the molecular system.

To understand the gradient-driven energy transfer we combine experiments -to determine the nature of the electronic excitation and energy transfer process- with computational results –to unravel the kinetics and intramolecular energy redistribution mechanism-. Through this joint effort, we find that the energy-transfer mechanism involves the ultrafast collapse of the photoexcited wavefunction due to non-adiabatic electronic transitions. Efficient coupling to high-frequency vibrational modes leads to ultrafast excited state dynamics and unidirectional efficient energy funneling.

To advance beyond this fundamental understanding, we explore new dendritic molecules that can further expand the applications of dendrimers in photoactive devices. Conjugated Polyelectrolyte Dendrimers are macromolecules with weakly coupled π-conjugated segments surrounded by ionic groups. A combination of chemical substitution and conjugation length yields dendrimers with energy gradients that biased the vectorial energy transfer towards their core. Time-resolved fluorescence characterizes the efficient energy transfer showing a reduction on the quantum yield with faster rates for energy transfer in the ionic macromolecules. These faster rates combined with lower quantum yield are attributed to smaller contribution to this process from the outer phenylene-ethynylene units of the dendrimers.

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A density-difference-driven optimized embedding potential method to study spectroscopy of Br_2 in water clusters and clathrate cages

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A density difference driven optimized embedding potential (DDD-OEP) method is proposed to obtain embedding potentials to calculate excited electronic states in large systems. This method considers the partition of the density of a system in two portions. The density on each subsystem is the solution of a Fock equation modified by the addition of an "embedding" potential. This embedding potential is obtained iteratively by minimizing the difference between the electronic densities of the total system and the sum of the subsystems [1,2].

This method is applied to study the electronic excitation of the Br_2-H_2O complex[3] where exact calculations are feasible[4]. It is found that the embedding potential for the ground and electronic states are different to properly describe the energy excitation, because the orbitals involved in the electronic excitation also participate in the forming the complex in the ground electronic state. A similar situation is found for the Br_2-$(H_2O)_n$ complex. On the relatively large $(H_2O)_{24}$ clathrate cage the water-halogen binding is considerably weaker and the excitation energy found using one unique embedding potential seems reasonable, waiting for more accurate benchmark. A diagnosis method, based on the analysis of initial density-difference is proposed to determine whether or not a single embedding potential is able to describe electronic excitation on large systems.

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Relaxation dynamics in quantum dissipative systems: the microscopic effect of intramolecular vibrational energy redistribution

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We investigate the effect of inter-mode coupling on the vibrational relaxation dynamics of molecules in weak dissipative environments. The simulations are performed within the reduced density matrix formalism in the Markovian regime, assuming a Lindblad form for the system-bath interaction. The prototypical two-dimensional model system representing two CO molecules approaching a Cu(100) surface is adapted from an ab initio potential, while the diatom-diatom vibrational coupling strength is systematically varied. In the weak system-bath coupling limit and at low temperatures, only first order non-adiabatic uni-modal coupling terms contribute to surface-mediated vibrational relaxation. Since dissipative dynamics is non-unitary, the choice of representation will affect the evolution of the reduced density matrix. Two alternative representations for computing the relaxation rates and the associated operators are thus compared: the fully coupled spectral basis, and a factorizable *ansatz*. The former is well-established and serves as a benchmark for the solution of Liouville-von Neumann equation. In the latter, a contracted grid basis of potential-optimized discrete variable representation is tailored to incorporate most of the inter-mode coupling, while the Lindblad operators are represented as tensor products of one-dimensional operators, for consistency. This procedure results in a marked reduction of the grid size and in a much more advantageous scaling of the computational cost with respect to the increase of the dimensionality of the system. The factorizable method is found to provide an accurate description of the dissipative quantum dynamics of the model system, specifically of the time evolution of the state populations and of the probability density distribution of the molecular wave packet. The influence of intra-molecular vibrational energy redistribution appears to be properly taken into account by the new model on the whole range of coupling strengths. It demonstrates that most of the mode mixing during relaxation is due to the potential part of the Hamiltonian and not to the coupling among relaxation operators.

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Recent developments in quantum reaction dynamics: from normal- to extreme-time regimes

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This talk has two parts. The first addresses the *ab initio* calculation and modeling of the potential energy surface(s). The importance of accurately describing both the ubiquitous van-der-Waals interactions [1] and chemical bonding, in addition to other topographical features such as crossings of the conical type is noted, and recent progress towards such forms discussed: analytic vs numerical, single- vs multi-sheeted [2]. The second part of the talk focuses on quantum dynamical issues: (a) code for atom+diatom reactive scattering in hyperspherical coordinates, with novel results for the D^++H_2 reaction [3]; (b) photoelectron spectra of CH_4 and CD_4 by focusing on the fast rearrangement from the T_d structure of CH_4 to the equilibrium C_{2v} geometry of CH_4^+. Besides obtaining good agreement between the calculated and measured vibronic bands of CH_4^+ and CD_4^+, it is shown that the dynamics occurring at the triply-degenerate ground electronic manifold of CH_4^+ in the sub-femtosecond time scale can be studied with regular dynamics by simulating the ratio of the emitted high-harmonic signals [4]. Simplified schemes toward this goal are also examined. Prospective remarks conclude the talk.

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8th photo dynamics

Cold and controlled ion chemistry

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Recent advances in the preparation and manipulation of neutral molecules and ions at temperatures below 1 K have opened up new possibilities for the study and control of chemical reactions. Samples of cold and spatially localized ions in traps, often referred to as Coulomb crystals [1], are attractive systems in this context because they enable the study of reactive processes on the level of single particles. We will give an overview of recent results on reactive collisions between cold neutrals and ions using a “hybrid” trap, i.e., a trap for the simultaneous confinement of both species. We will illustrate the exotic chemical processes and the the chemical dynamics which occur in ion-neutral systems at extremely low temperatures [2]. We will also present first results from a recently developed “dynamic” hybrid trap experiment which enables the study of cold collisions and reactions with superior energy resolution. We will also highlight recent work on reactive collisions between Coulomb-crystallized ions and conformationally selected neutral molecules as a new method to study and control conformer-specific effects in bimolecular reactions of complex molecules [3]. The scope of this new technique will be discussed and future directions outlined.

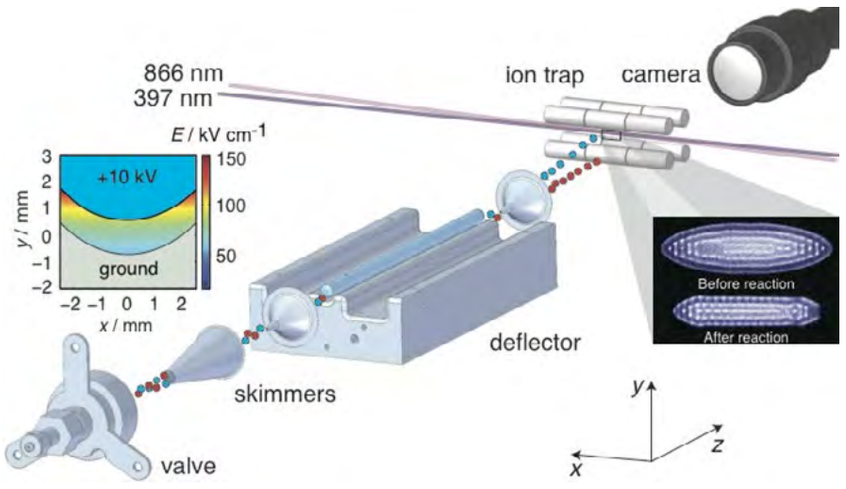

Figure 1. Experimental setup for the study of conformationally selected ion-molecule reactions [3].

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Ultracold Chemistry: Separation of Short-range and Long-range Dynamics

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The extraordinary progress achieved in recent years in cooling, trapping, and manipulating a variety of atomic and molecular species has opened up exciting opportunities for investigating chemical reactions in the extreme quantum limit. The ability to prepare molecules in specific spin and hyperfine levels and observe reactivity at the level of a single partial wave has spurred new interest in quantum control of chemical reactions. However, theoretical investigations of these processes are faced with significant challenges due to the proliferation in the number quantum states (vibration, rotation, spin, and hyperfine levels) to be included in the calculations. Due to large de Broglie wavelengths associated with ultracold collisions, radial integration of coupled-channel equations in quantum dynamics calculations needs to be performed over much larger molecular separations. Significant savings can be achieved if the short-range and long-range dynamics could be separated and a simplified formalism be used in the long-range. Here we present such an approach that combines quantum close-coupling at short-range with quantum defect theory at long range. The method yields full state-to-state rovibrationally resolved cross sections as in standard close- coupling calculations but at a considerably less computational expense. The method, illustrated for $D+H_2$ collisions with rovibrational quantum state resolution of the HD product, is shown to be accurate over collision energies spanning six orders of magnitude and a wide range of initial conditions.

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Rovibrational autoioinization in D_2 and H_2: a window to strong electron-core coupling in molecules

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In the region just above the first, $v^+ = 0$, ionization threshold, the photoionization spectra of both H_2 and D_2 are dominated by ro-vibrational autoionization [1]. This is a two-step process. A photo-excited neutral Rydberg state, converging on ro-vibrationally excited states of the ground electronic state of the molecular ion, may autoionize to a lower ro-vibrational state of the molecular ion by the transfer of some of the ro-vibrational energy to the escaping electron. The simple electronic structures and relatively large rotational spacings of H_2 and D_2 have made them the target of choice for experimental and theoretical studies of this ro-vibrational autoionization and this work has been summarized before [2]. In work we present experimental work on the photoionization of H_2 and D_2 aimed at studying the dynamics of the photoionization process of these molecules using synchrotron radiation and a high resolution, angle resolved photoelectron spectrometer. These studies have been carried out at the Gasphase at the Elettra Sinchrotron Source. The photoionization, near the ionization threshold of these small molecules, enables to study the Fano resonances arising from autoionizing processes induced by the coupling of the ro-vibrational transitionswith the ionization continuum. In addition to the photoionization yield as a function of initial, final and intermediate states, we are able to experimentally determine the asymmetry parameter of the angular distributions of the emmited photoelectrons. This particular example of molecular autoionization will be used as a base to discuss the general aspects of autoionization in molecules and atoms, first discussed theoretically by Fano in the context of the Configuration Interaction Picture. The specific example presented in the talk, pertaining the photoionization of D_2 will help to illustrate strong violations to the Born Oppenheimer picture in small molecules.

Acknowledgements: AM Juárez Acknowledges the support of CONACYT through the grant CB-2011 167631.

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Reactive scattering $^{87}Rb + {}^{87}RbHe \rightarrow Rb_2(^3\sum^+_u, v) + He$ at ultracold energies

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It has been suggested that rubidium atoms deposited on the surface of helium nanodroplets can collide at cold energies yielding molecular rubidium Rb_2 in excited vibrational levels of the (preferentially) ground triplet electronic state[1]. As a preliminary step to assess this possibility we study atom-diatom reactive collisions through an extremely simple model that extends the well-known Rosen treatment on linear triatomic molecules[2]. Using the best three-dimension potential energy surface available[3], and expressing the Hamiltonian of the system in satellite coordinates, the model allows one to estimate reaction probabilities and cross-sections at different values of the total angular momentum. These magnitudes numerically fulfill the Wigner threshold laws. The efficiency of the reactive process is enhanced at ultracold collision energies for a total angular momentum J=1, as occurs in recent studies on vibrational relaxation of rubidium dimer by collisions with helium atom[4]. The Rb_2 product is essentially formed at vibrational states $v \geqq 25$. Also, one finds that the boson ^4He atom as partner is more efficient than the fermion one to produce the rubidium dimer.

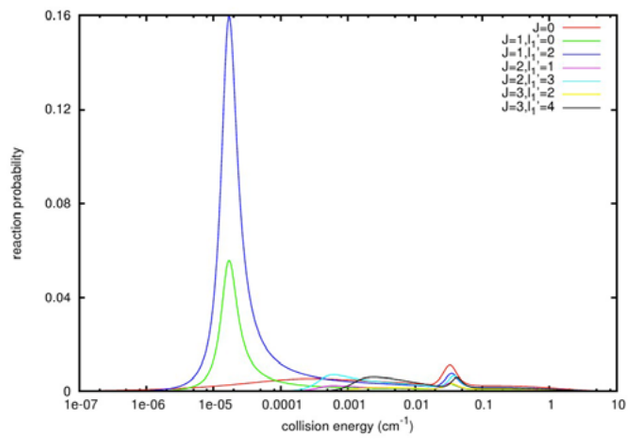

Figure 1. For ^4He partner, probabilities of Rb_2 formation in different reaction channels.

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Enhancing mechanisms of optical activity of chiral molecules adsorbed in metallic nanoparticles

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It has been observed that ligand-protected metallic nanoparticles have an exceptional optical activity that is contrasting to those of the components: ligands and nanoparticles. Adsorption of organosulfur (SR) molecules on metal NPs could offer the possibility to create strong optical activity in the visible región. Circular dichroism (CD) is a preferred tool for characterizing optical activity of chiral systems, which measures slight differences existing in optical extinction between left and right circularly-polarized light passing through chiral substances. CD has a moderate sensitivity, which hampers the analysis at low concentrations and/or low enantiomeric excess. Controlled CD signals from organic molecules by using metallic NPs is desirable for having an enhancement mechanism of the optical activity. The latter might improve chiroptical spectroscopic techniques, which are useful to study molecule-molecule and molecule-nanostructure chiral interactions, which are of great significance since most molecules relevant in life are chiral. Thus, organometallic compounds have emerged in recent years as interesting nanoscale systems that hold promise in a wide range of applications, including molecular recognition.

Enhancement of the CD spectra coming from the ligands has been observed to increase as the size of Ag NPs does. To explain this, it has been proposed that surface plasmons supported by the metal NP enter in resonance with electronic transitions of the ligands involved in optical activity. However, it is not clear until now how much this effect enhances the signal from the molecule, and even more if this is the only mechanism. There might be other factors associated to NPs and ligands that could contribute besides NPs size. For example, as the NP size increases the number of ligands adsorbed on it also does, and an augmentation of the CD signal is expected. However, there are other subtle effects that are related to the structure and bonding of the metallic NP and the molecule.

In this talk, we are interested in explain how the metallic nature of the NP, the number of adsorbed ligands, and the geometrical properties influence the chiroptical signals that can be seen as possible CD enhancement mechanisms.

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Dynamics of atom-diatom reactions at the low energy regime

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The dynamics of some atom-diatom reactions has been investigated in the low collision energy regime (E_{coll} < 10^{-1} eV). The possibility of complex-forming mechanisms is analyzed by means of a statistical quantum method [1,2] in comparison with quantum mechanical results and experimental measurements. The case of the $H^+ + H_2$ reaction, and isotopic variants, for which a significant dependence on the energy range has been reported before, is treated in detail [3], Recent studies on the $D^+ + H_2$ reaction found theoretical rate coefficients in a good agreement with experiment down to 10^{-3} eV [4,5]. Similar investigations in other reactions such as Li+YbLi and $He+NeH^+$ [6] are discussed.

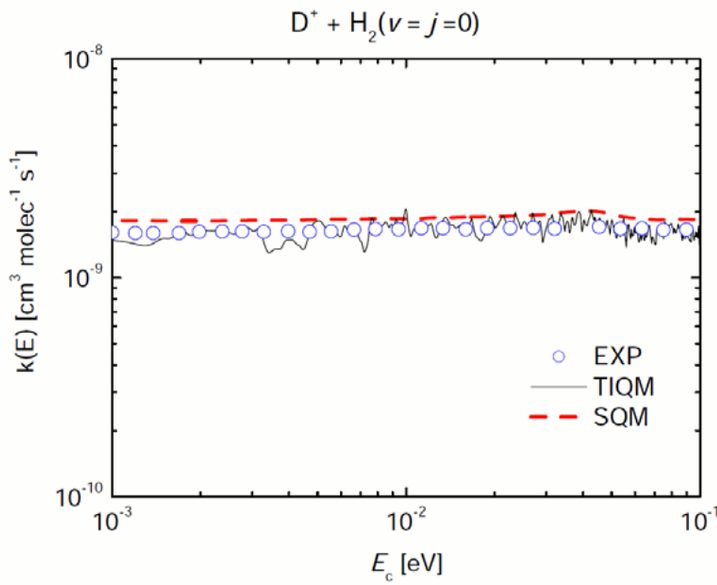

Figura 1. Rate coefficient for the $D^+ + H_2 \rightarrow HD+H$ reaction. A comparison of statistical, time independent quantum mechanical and experimental results.

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Strong-Laser-Field Control of Ultrafast Photochemistry

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Strong-laser-field control scenarios of ultrafast molecular photodissociation dynamics are presented. The control is exerted on different observables of the photochemical reaction, such as quantum yields and lifetimes or even on fragment kinetic energies. The control is achieved by opening new strong-field-induced reaction channels [1] or by creating light-induced-conical-intersections and modulating the potentials around them by light-induced potentials [2]. The case study involves photodissociation of the polyatomic prototype methyl iodide (CH_3I), whose ultrafast photodissociation dynamics has been studied in our laboratory for some years both in the *A*-band [3,4] and *B*-band [5,6].

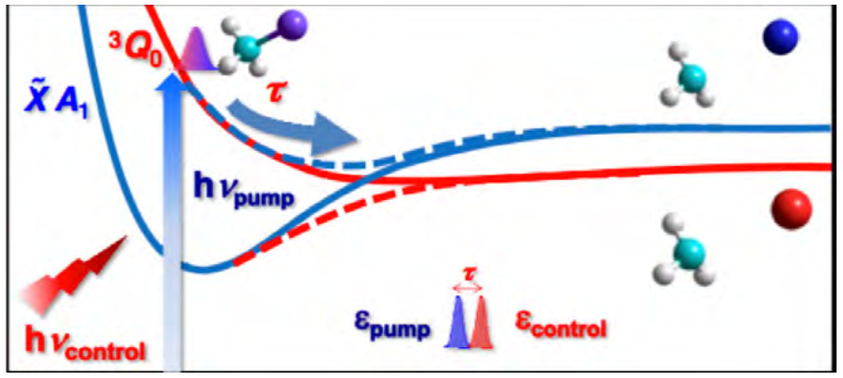

Figure 1. Shaping potential energy surfaces by tailored strong laser pulses is a powerful means for controlling product yields. Control over the velocity of the product fragments is achieved through the generation of light-induced conical intersections and modulating the potentials around them by creating light-induced potentials.

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Analyzing the Binding of Positrons to Atoms and Molecules with the Any Particle Molecular Orbital Method

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Abstract. A number of theoretical methodologies developed within the any particle molecular orbital approach [1], APMO, have been applied to study positron bonding to atoms and molecules [2-3]. Our results show that the APMO approach is a reliable and affordable alternative to study the nature of the interaction of positrons with molecules.

Keywords. APMO, positrons

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Electronically Induced Dynamics from Atomistic Simulations

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Empirical force fields are a powerful means to investigate the long-time dynamics of molecular systems. For a meaningful description of experimental observables, suitable forms of the energy function and their accurate parametrization are required. In this contribution I will present force field methods for metal-containing systems and how they can be applied to characterize, at atomic resolution, the dynamics of ruthenium- and iron-containing complexes. The computational model is based on valence-bond theory (the VALBOND and VALBOND-trans force fields) which has been developed in order to describe the unusual angular dependence of the total energy in metal-containing systems. Furthermore, the solvation and proton-transfer dynamics in an industrially relevant platinum-complex is presented.

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Dynamics of the High-lying Singlet Excited States of Polymethinic Compounds

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The electronic relaxation dynamics of the upper singlet excited states S_n (n>1) of polymethinic cyanine dyes was investigated. The population decay of these states was monitored for a set of nine dyes through the femtosecond fluorescence up-conversion technique. It was observed that for several of the cyanines, the S_2 state is unusually long-lived with decay rates as small as $5x10^{10}$ s^{-1}.[1] The dynamics after electronic excitation to singlet states above the fluorescent state actually varies significantly as a function of cyanine structure. For example, while all the cyanines in the 2-quinolyl series have S_2 decay times in the subpicosecond regime (<0.2 ps), several dyes in the thia-carbocyanine family, like 3,3'-diethyl-2,2'-thiatricarbocynane, have long-lived S_2 states (17.3±0.1 ps). Compounds 4-quinolylcyanine and 2-quinolylcyanine (with a single methinic carbon bridge and non-planar geometries) also have ultrafast S_2 decay times, however, for the rest of the cyanines (with nearly planar geometries), we observed a trend in the upper state decays that closely follows the energy gap law. It was further demonstrated that the long-lived S_2 singlets can also be efficiently formed by degenerate two photon absorption with near IR femtosecond pulses. The present study isolates the structural variables that determine the lifetimes of the second singlet states (S_2) in polymethinic compounds. Our interest in these molecules comes from the potential applications of two-photon sensitizers with atypically long S_2 lifetimes, which may allow processes of energy or electron transfer before relaxation to the first singlet excited state.[2]

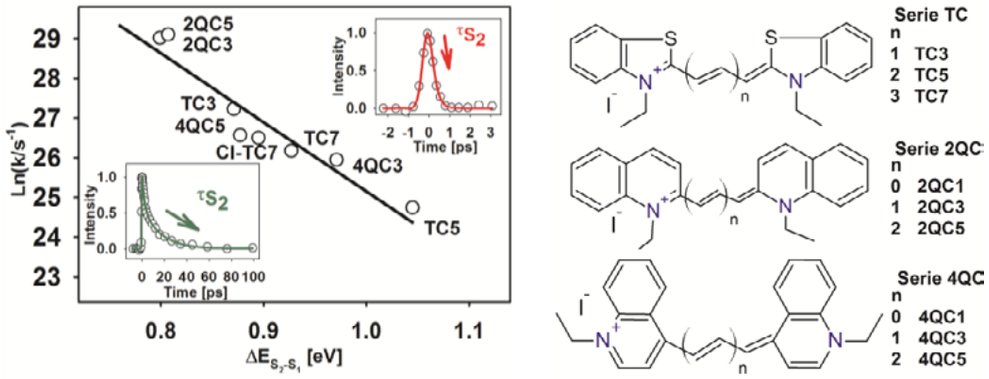

Figure 1. S_2 decay rates as function of the energy gap between S_2–S_1 excited states of the cyanine dyes. Structures of cyanine dyes for this study.

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Theoretical study of the Si + OH → SiO + H reaction

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Reactions between pairs of neutral radicals are important for the chemistry of the interstellar medium (ISM). They occur rapidly and, due to the absence of energy barriers, they can proceed efficiently down to the low temperatures prevailing in the ISM. In particular, the reaction between the hydroxyl radical OH and the open-shell Si atom is thought to be a major source of SiO, one of the most useful tracer of shocked gas in star-forming regions. The lack of reliable kinetics data for this process has prompted us to perform a detailed theoretical study of the dynamics of the Si+OH reaction. A global potential energy surface (PES) has been developed [1] for the ground X^2A' electronic state of the SiOH/HSiO system, which correlates adiabatically to the products SiO+H. The PES is based on ab initio energies computed from the multireference configuration interaction (MRCI) method with basis sets of quadruple zeta quality, complemented by the results of perturbation theory to represent the Si+OH long-range interactions [2]. The quasi-classical trajectory (QCT) and time-dependent wavepacket (TDWP) methods were employed to treat the reaction dynamics. The TDWP calculations were performed for a total angular momentum J=0, and the J-shifting approach was used to evaluate the contribution to reactivity of J>0 partial waves. We will present the main features of the X^2A' PES and the most recent results [3] obtained for the state-selected cross sections, rate constants, and product state distributions of the title reaction.

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Fragmentation dynamics of NO–NO dimer: A quasiclassical dynamics study

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The quasiclassical trajectory method is applied to the vibrational predissociation of the NO(r)–NO complex. A new ab initio potential energy surface was used within a reduced dimensionality mode[1]. A metastable resonance state of the complex is prepared, for different intramolecular and intermolecular modes. Among the unique and interesting features of this system is the presence of many bound intermolecular modes with strongly varying predissociation properties and a strong vibration–translation coupling. Our calculations are in good agreement with the measured experimental lifetimes for the fundamental and overtone excitation of the antisymmetric stretch and bring support to a vibrational coupling mechanism[2]. We are comparing our previous studies with more recently ones using Wigner distributions in order to get the initial conditions.

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Seeing the chemical bond in motion, in an ensemble, and in solo

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The most complete moving images of the chemical bond in motion, of bromine doped in ordinary ice, has been recorded through electronically resonant four-wave mixing measurements. The measurements allow a tomographic state reconstruction, and determination of the time dependent Wigner distribution function (WDF) of a bond undergoing dissipative dynamics in an open system. The non-classical nature of the motion is manifested by the negative volume of the WDF - a first time observation in ordinary molecular matter. Spectral decomposition of the WDF yields the tomograms of individual coherence terms in phase space, which in turn yield the wavefunctions of the evolving states. Indeed, we see the wavefunctions.

Quantum dynamics in ensembles is limited by decoherence, which marks the transition to classicality. There is no such limit for coherences prepared on single molecules. They may acquire phase noise due to the inescapable environment, but they do not undergo pure dephasing. This, we recently demonstrated in the first time-resolved measurements of a vibrational coherence prepared and interrogated in a single molecule. To reach single molecule sensitivity, we employed time-resolved, surface-enhanced, coherent anti-Stokes scattering on a bipyridyl-ethylene molecule equipped with a Hertzain dipole nano-antenna (gold nanosphere dimer). The preparation and interrogation of coherences in single molecules suggests many new applications in molecular photonics. By force of being single, the molecular interactions and signals obey quantum statistics.

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Real space techniques to understand chemical bonding in excited states

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The theory of the chemical bond has focused in the past in understanding ground state properties of chemical systems, leading to a set of well-defined rules dominated by the molecular orbital (MO) paradigm. Bonding and reactivity in excited states, being intrinsically more complex than the dynamics of ground states, have received much less attention in the specialized literature. In the end, our comprehension of these phenomena is still based on one-electron MO pictures. During the last 30 years, orbital invariant real space theories of the chemical bond have become a clear alternative [1] to MO thinking. These mehods are usually known as topological theories of the chemical bond, the Quantum Theory of Atoms in Molecules (QTAIM) developed by R. Bader possibly being the best known example. The QTAIM has all the features that might be useful in excited state dynamics: it does not depend on the underlying computational scheme; it is able to provide results both in systems where electron correlation is not an issue as well as on those where multi-reference effects are essential; etc. However, a long prejudice dating back to the 1980's on the inability of this technique to tackle with excited states as well as with non-equilibrium geometry has precluded the application of the theory to excited states. All these prejudices are being debunked: excited states quantum atoms are perfectly valid in the vast majority of cases, and general energetic partitions [2] within the theory allow for examining both equilibrium and non-equilibrium molecular geometries. We present here a simple account of the QTAIM framework to the photodynamics community, showing how it may be useful in understanding excited state reactivity and dynamics. A few examples [3,4] will also be discussed.

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Protonated hydrogen clusters PES and Dynamics

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Results of recent studies on the H^+_{2n+1} clusters will be presented. Nowadays high accurate ab initio electronic structure calculations can be carried out [1]. An alternative DFT approach using the B3(H) hybrid functional allows to carry out reliable dynamics calculations, by computing the potential value at a given configuration, on the fly, with both reasonable accuracy and at low computational cost [2]. Based on this surface both classical and path integral Monte Carlo (CMC, PIMC) calculations at low temperature are carried out to investigate quantum effects on the internal proton transfer and thermal structural fluctuations on the vibrational zero-point structure of H^+_5 cluster. Full-dimensional (9D) multiconfiguration time-dependent Hartree (MCTDH) computations are reported for the vibrational states of the H^+_5 and its deuterated isotopologues [3]. It is found that these systems are highly delocalized, interconverting between equivalent minima through rotation and internal proton transfer motions. Isotopic substitution affects the zero-point energy and structure, showing preference in the arrangements of the H and D within the mixed clusters. Several vibrationally excited states are presented and analyzed [4]. Finally, reduced dimensional quantum dynamics calculations of the infrared spectrum of the H^+_5 and D^+_5 clusters are reported [5].

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8th photo dynamics

Weakly-bound molecular complexes formed from three- and four-atom linear molecules

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During the past few years, our group has been systematically investigating the infrared spectra of weakly bound dimers and larger clusters formed from CO_2, N_2O, OCS, CS_2 and C_2H_2. The aim is to probe the intermolecular forces in these systems by providing clear spectroscopic data against which theory can be benchmarked. As well, results on trimers, tetramers, and larger clusters may give insight into nucleation and condensation dynamics and into orientational disorder effects in molecular crystals. Each size of a cluster may have multiple isomers and may also have multiple vibrational bands corresponding to a given monomer vibration.

Our spectrometer is a pulsed supersonic jet apparatus. The expansion gas is probed using radiation from a quantum cascade, a Pb-salt tunable diode laser, or an optical parametric oscillator with all three lasers employed in a rapid-scan signal averaging mode. Multi-passing of the laser beam is accomplished using a toroidal mirror system (nominally 182 passes). The spectra are averaged typically for 500 to 4000 jet pulses. Our experimental technique does not give precise cluster size resolution. So the assignment and analysis of successive dimer, trimer, etc., bands is a synergistic process in that each newly assigned band helps “peel away” the total observed spectrum and to reveal further bands which may be partly hidden underneath. In this talk, I will describe the spectrometer and show some examples of spectra belonging to dimers, trimers, tetramers, and higher clusters formed from the molecules mentioned above.

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Adiabatic and Nonadiabatic Dynamics of CH($X^2\Pi$)+H(^2S) and Deuterated Reactions

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We present the quantum dynamics of the CH decays CH($X^2\Pi$)+H'(^2S)→C(^3P/^1D)+H_2($X^1\Sigma^+_g$) and H-H' exchange CH($X^2\Pi$)+H'(^2S)→CH'($X^2\Pi$)+H(^2S) on three PESs, coupled by nonadiabatic conical-intersection (CI), Renner-teller (RT), and spin-orbit (SO) effects shown in Fig. 1. Deuterated species are also considered. Using the real wavepacket and flux methods, we find that SO effects are negligible, and that the $\tilde{X}\,^3A$" dynamics is well described by the Born-Oppenheimer (BO) approximation, whereas other collisions occur with significant RT effects, as Fig. 2 shows for some reaction probabilities.

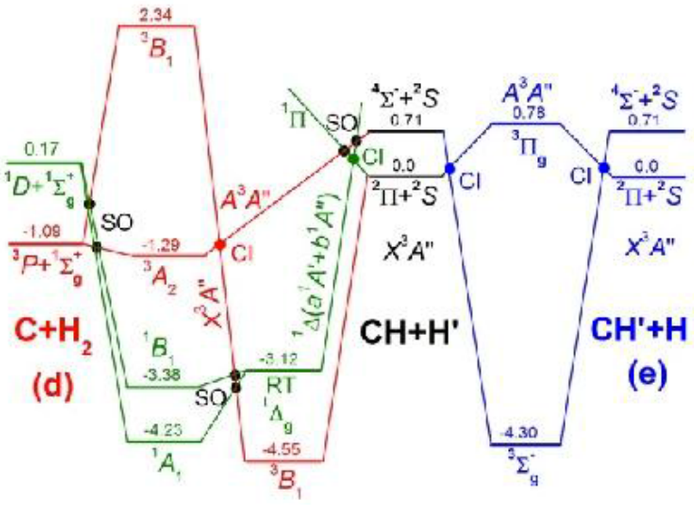

Fig. 1. Correlation diagram

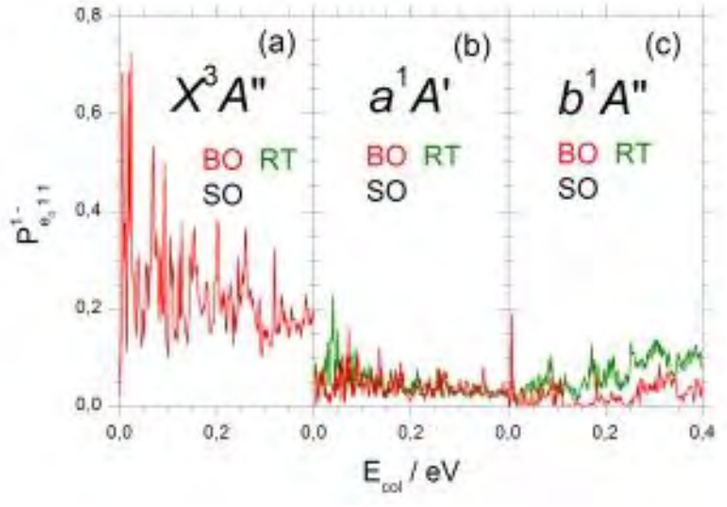

Fig. 2. BO, RT, and SO reaction probabilities

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Efficient Nonadiabatic Molecular Dynamics Rate Theory

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There is currently much work on the development of computationally practical methods for the simulation of nonadiabatic dynamics based on classical trajectories and path integrals such as ring-polymer molecular dynamics (RPMD) [1-4]. An important goal for such methods is the accurate calculation of the rate constant over a wide range of electronic coupling strengths without the need to approximate the potential energy surfaces by harmonic oscillators, as is commonly the case for less general methods. It is often the nonadiabatic, weak-coupling limit, which being far from the Born- Oppenheimer regime, provides the greatest challenge to current methods. For instance, the standard implementation of surface hopping gives a rate proportional to the electronic coupling, Δ, rather than the correct result, Δ^2, in this limit [5].

We show how nonadiabatic RPMD dynamics [1], based on the rigorous mapping approach [6,7] can be used to compute the rate of electron-transfer in complex molecular systems giving results which interpolate correctly between the golden-rule and adiabatic limits. This approach is not, however, efficient in the weak-coupling regime as the flux correlation functions become very oscillatory. We derive a generalization of the nonadiabatic flux correlation function [8], from which the rate can, in principle, be computed exactly regardless of the coupling strength, but which unlike the usual version is not oscillatory. This new formalism thus provides a rigorous way for a wide variety of methods from trajectory- to wavefunction-based approaches to calculate the nonadiabatic rate more efficiently. We present results of the mapping dynamics method with the new flux correlation function formalism for systems with weak electronic coupling including those in the Marcus inverted regime.

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8th photo dynamics

Photochemistry at the Surface of Cloud Water Droplets

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Photolysis reactions are central to atmospheric chemistry. Ozone in particular, absorbs UV and visible light and photodissociates to produce molecular and atomic oxygen either in the ground or excited states. Atomic oxygen can then react with water or methane molecules to form the highly reactive hydroxyl radicals OH, often referred to as the “detergent” of the troposphere. These processes have been widely investigated in the gas phase. However, ozone can be adsorbed by the surface of cloud water droplets and it is important to study the implications of this interaction in terms of spectral shifts and/or modification of the absorption cross sections. In a series of recent studies [1-4] we have developed a methodology to investigate chemical processes at water interfaces using combined QM/MM Molecular Dynamics simulations [5]. In this lecture, we will discuss recent results obtained for the photolysis of ozone [6] (Figure 1).

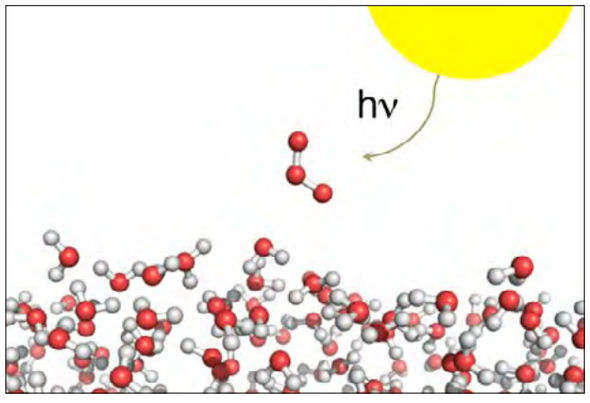

Figure 1. Snapshot from the QM/MM Molecular Dynamics simulation of ozone at the air-water interface.

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Rydberg Tagging of Spin-Polarized H atoms

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The production of spin-polarized hydrogen atoms produced in molecular photodissociation was considered theoretically more than thirty years ago [1], however it has been experimentally observed only recently, first by inferring based on the measured co-fragment angular momentum polarization [2], and subsequently by detection of the polarized fluorescence in the H atoms excited by Lyman-alpha radiation [3]. We present a new experimental technique allowing for direct measurement of the velocity dependence of hydrogen atom spin polarization with high resolution and sensitivity. The strategy is an adaptation of the H atom Rydberg time-of-flight approach (SP-HRTOF), where the spin-sensitive probe scheme combines a linearly polarized Lyman-α laser, a circularly polarized tagging laser, and a photolysis laser [4]. The approach is illustrated with a measurement of the H atom spin polarization in photodissociation of HBr and DBr at 212.8 nm. The two coherent contributions to the spin polarization are measured for H atoms produced in conjunction with dissociation to Br($^2P_{3/2}$) and Br*($2P_{1/2}$); they are found to be negligible for the former channel but substantial for the latter, in agreement with previous theoretical predictions. The ratio of the two measurements directly gives the asymptotic scattering phase shift for dissociation along the two potentials for the H + Br* channel. The paper also discusses the means to adapt this method to detect the incoherent contribution to the photofragment spin polarization, and discuss our progress in applying the technique to dissociation of polyatomic molecules.

The present results show the capability for SP-HRTOF to yield fundamental insights into molecular scattering processes. Applications to dissociation of polyatomic molecules and reactive and inelastic scattering promise a wealth of new detail concerning these elementary processes.

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Recent progress in description of water from first principles

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A force field for water, developed by our group completely from first-principles, achieved a description of all forms of water, from the water dimer to liquid water, at accuracy levels comparable to those of the best measurements (Science 315, 1249 ‘07). Several advances since this work will be described. The 2007 force field was improved both at the two-body level (PCCP 10, 4716 ‘08) and the three-body level (JCP 140, 194101 ‘14) by using higher levels of theory in calculations of interaction energies, larger numbers of grid points, and more flexible fitting functions. Although this force field still assumes rigid monomers, it gives better predictions for water clusters that the predictions from the best published flexible-monomer force fields. At the two-body level, our group has developed a force field with flexible monomers (LSCCS 6, 482 ‘06, JCP 137, 012305 ‘12), needed for predicting properties such as shifts of monomer vibrational frequencies upon dimerization. The virial coefficients for water obtained accounting for both monomer flexibility and quantum effects challenge the experimental determination of this quantity. With our very accurate two-body component, we have examined (JCP 138, 024316 ‘13) how well the polarization model of many-body nonadditive forces can describe the liquid water. This model is commonly used, despite several papers showing that it reproduces three-body nonadditive effects rather poorly. In our calculations, the average error of this model relative to accurate *ab initio* values of three-body interaction energies for a large set of trimers selected from simulations was as large as 71%. A more in-depth analysis, taking into account the fact that the errors gradually decrease for larger trimers, allowed us to estimate, however, that despite this problem, the polarization model should be capable to reproduce the exact liquid water interaction energy to within about 6%, consistent with the observed performance of this model relative to experiment. For several observables, the use of the polarization nonadditive forces leads to a dramatic improvement of the agreement with experiment compared to the use of the virtually exact two-body potential. Apparently, the reason is that whereas the two-body forces alone produce an unstructured liquid, the polarization nonadditive forces are just sufficient to restructure it into tetrahedral arrangements.

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Molecular modeling of organic coated sea-salt particles

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The aerosol and gases in the atmosphere play an important role on health, air quality and climate, affecting both political decisions and economic activities around the world [1]. Among the several approaches of studying the origin of these effects, computational modeling is of fundamental importance in providing insights on the elementary chemical processes. Sea salts are the most important aerosol particles in the troposphere (10GT/year) [2]. Our theoretical work consists in modeling a (100) NaCl surface coated with palmitic acid (PA) molecules, the most abundant fatty acid present in second organic aerosols. Different PA coverages have been studied with varying the degree of humidity. A transition in the molecular orientation of the adsorbate has been evidenced. The trends obtained from the calculations are compared to experimental results [3] and their implications for atmospheric chemistry are discussed.

Acknowledgments: this research has been supported by the CaPPA project (Chemical and Physical Properties of the Atmosphere) [4], funded by the French National Research Agency (ANR) through the PIA (Programme d'Investissement d'Avenir) under contract ANR-10-LABX-005.

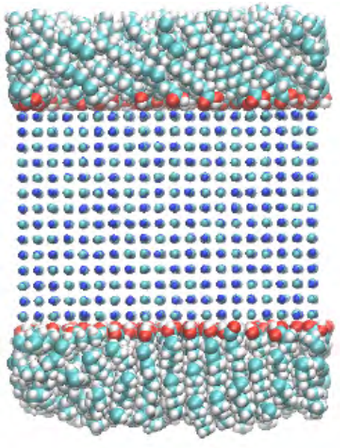

Figure 1. Coating of the NaCl surface by a palmitic acid layer.

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Theoretical study of the photodetachment of the negative ions of reaction intermediates

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Neumark and co-workers have pioneered the use of photodetachment spectroscopy to investigate the potential energy surfaces of the paradigm $F+H_2$ [1,2] and $Cl+H_2$ [3] abstraction reactions. The use of slow photoelectron velocity map imaging and precooling the anion [4] allows enough resolution to resolve resonances arising from quasi-bound reactant or product states. This technique provides information on the reactive potential energy surface complementary to that obtainable from crossed molecular-beam studies.

We shall present new calculations for the FH_2 system based on two recent potential energy surfaces [5–7], and compare our predicted spectra with recent experiments by Weichman and Neumark. Also, we shall discuss similar ongoing investigations of the photodetachment of the $ClCH_4^-$ and SD_2^- complexes.

Time permitting, we will describe recent work in which the investigation of the relative reactivity of the ground and excited states of Cl with H_2 [8] is extended to higher energy.

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8th photo dynamics

Time-resolved radiation chemistry: interaction of low energy electrons with nucleobases

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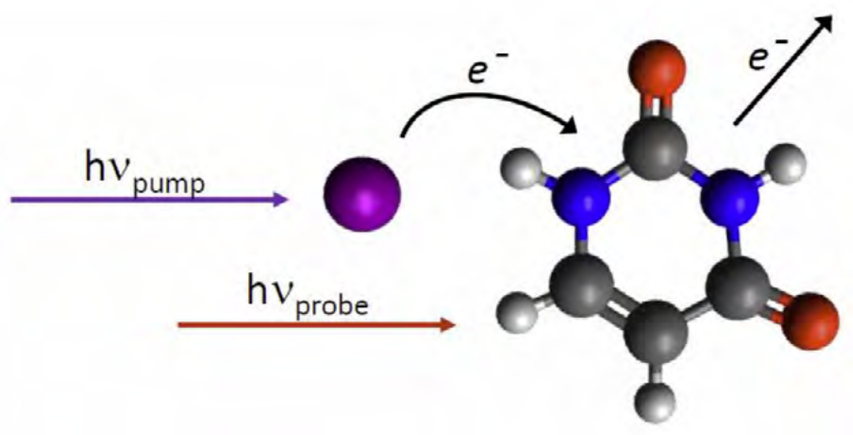
The interaction of low-energy electrons with nucleic acid constituents plays a key role in radiation chemistry and biology. In our laboratory, we investigate the dynamics of this interaction via femtosecond time-resolved photoelectron spectroscopy. Experiments thus far have been carried out in the gas phase on binary iodide-nucleobase clusters. Here, a femtosecond pump pulse ejects an electron from the iodide anion, which is then captured by the adjacent nucleobase to form a temporary negative ion (TNI). The time- resolved formation and decay of the TNI is characterized by photodetachment with a femtosecond probe pulse and measurement of the resulting photoelectron spectrum. Planned experiments include carrying out measurements of this type on nucleic acid constituents dissolved in liquid water microjets.



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Optical trapping: From non-linear dynamical systems to optical solitons

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Optical trapping and manipulation of microscopic objects with laser light is nowadays a well-established technique. In the simplest case of a Gaussian light distribution, the gradient optical force attracts transparent dielectric particles towards the maximum intensity region when their refractive index is higher than that of the host medium. For other kinds of complex intensity distributions, however, like a set of periodic fringes, the optical force and the associated potential depend on the size of the particle with respect to the characteristic size of the light pattern. This fact can be used to design versatile experimental models of mechanical systems by tailoring special light distributions and choosing the size of the microparticles interacting with light. On the other hand, when the size of the particles is well below the wavelength of the trapping beam, as in a suspension of nanoparticles, the medium behaves as an effective medium with non-linear optical properties owed to the gradient optical force. Both these limits will be briefly discussed.

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Time-Resolved White-Light Spectroscopy and Optimum Control of Metal Clusters

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In our project we identify optical pathways that connect initial molecular configurations via a series of excited states to a chosen target state of desired charge, structure and function. For this purpose we employ spectrally and temporally shaped white light laser pulses which drive the system across a series of temporally opening and closing Franck-Condon windows to reach the desired target state. The initially ultrafast (<5fs) white light pulses are extracted from plasma filaments [1]; the described ladder climbing process is optimized in feedback loops, which are based on genetic algorithms. As a result, the initially non-resonant multi-photonic transition becomes resonant, making it significantly more efficient and much more selective.

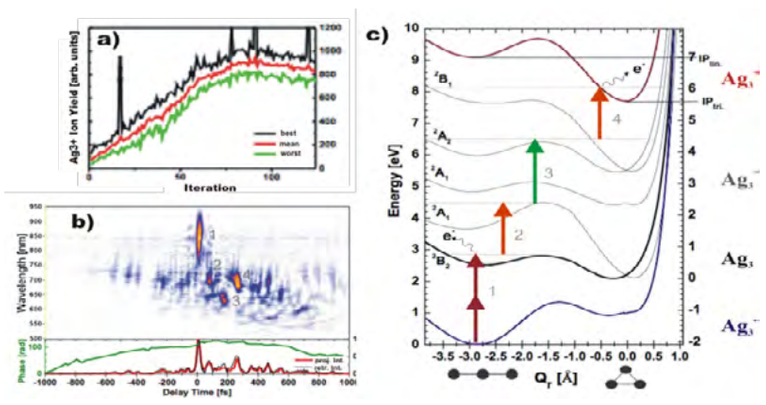

Figure1: Results obtained from the charge reversal process of Ag_3 [2]. Insert a) shows learning curves. The spectral and temporal behavior of an optimized pulse sequence is shown in insert b). The numbered segments of the resulting pulse train are depicted again at the corresponding locations of insert c), where the positions of the potential energy curves for Ag_3^{-0+} are given.

The transitions shown in figure1 indicate a ladder climbing process, which starts with the linear molecule Ag_3^-. First the particle is photo-detached; then it climbs along various electronic states of neutral Ag_3^*, ending up in the structure of the equilateral triangle of Ag_3^+. More examples, as obtained from Cu_3 and Al_3, will be presented and their possible use in optically driven nano-engines will be discussed.

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8th photo dynamics

Excited State Dynamics of Isolated Nucleobases

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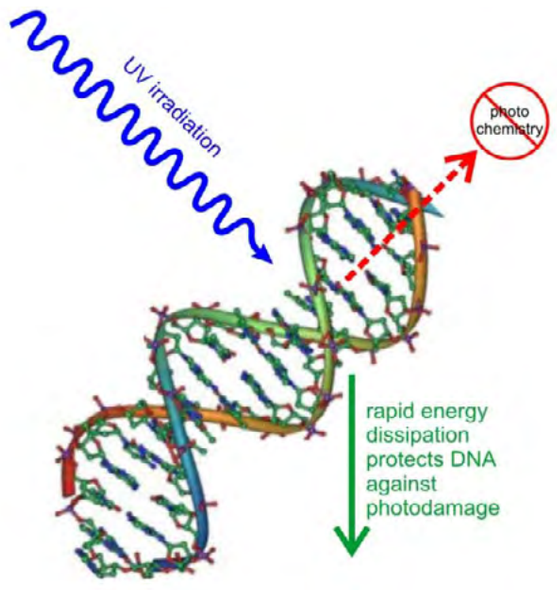
From a chemical perspective one may define the origin of life as the synthesis of the first macromolecule with a replication scheme, such as RNA. Today's extensive biochemical machinery, involving complex proteins and enzymes, would not have existed on a prebiotic earth, before life started. Therefore we investigate the fundamental properties of nucleobases without the contemporary biological environment by studying them as *isolated* molecules and clusters, in the gas phase, generated by laser desorption and employing double resonant spectroscopy.

We report on the results of IR-UV hole burning spectroscopy of nucleobases, nucleobase derivatives, nucleosides, and their clusters with each other, as base pairs, and with water. In combination with *ab initio* modeling a picture emerges in which most of the heterocyclic compounds that today are involved in replication exhibit UV photochemical stability by virtue of sub-picosecond excited state life-times. In many cases other derivatives, tautomers or structures of *the same compounds* do not exhibit this mechanism, rendering them much more vulnerable to UV radiative damage. This suggests the possibility of a photochemical selection of the molecular building blocks of life, as we know it, long before the advent of biological selection. It is thus conceivable that the molecular properties of nucleobases, which we study, are relics from prebiotic chemistry, 4 billion years ago.



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Connection Between the Upper and Lower Energy Regions of the Potential Energy Surface of the Ground Electronic State of the HSO_2

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The importance of the HSO_2 system in atmospheric chemistry has motivated several works dedicated to the study of associated structures and chemical reactions. Nevertheless, controversy still exists about a possible connection between the upper and the lower energy regions of the potential energy surface (PES) for the ground electronic state of the system. Previous attempts at finding a transition state connecting the two regions have failed [1-3]. Recently [4] a path to connect these regions was proposed based on studies at the CASPT2 level, using a global double many-body expansion PES (DMBE) [2]. However, the small energy difference between some of the transitions states along the path suggested the need of calculations at a higher level of theory. In this talk we present a CCSD(T)/aug-cc-pV(T+d)Z study of the stationary states associated to the proposed connection path, including assessment of the most reliable complete basis set (CBS) extrapolation scheme for the system. The results of the calculations [5] showed that the structures relevant to the proposed connection path belong to different electronic states. The presence of crossing seams has been confirmed by SA-CASSCF calculations. In conclusion, the calculation show that there is indeed a connection path between the upper and lower regions which allows the reaction $SH + O_2 \rightarrow H + SO_2$ to take place but that this path involves two conical intersections which must be taken into account when using the DMBE to perform dynamic calculations. (CNPq, FAPERJ)

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Excited molecules on the verge of a triple breakdown: roto-vibrational roaming roads

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Advances in studies of dissociations of excited molecules are revealing unexpected mechanisms when their outcomes are approached by combining imaging in space and time of translational features with spectroscopic probing of rotational and vibrational distributions; crucial is the assistance of quantum chemical investigations of selective rupture of chemical bonds and of molecular dynamics simulations of the evolution of their break up. Alternative pathways in chemical kinetics are repeatedly being discovered [1,2], and such a multiplication of reports urges molecular scientists to turn their attention to regions of the potential energy surfaces other than those in the neighborhoods of saddle points along minimum energy paths: eventually this will lead them to avenues beyond the venerable transition state approach [3].

Here we present an integrated experimental and theoretical approach [4] applied to the simplest ester, methyl formate $HCOOCH_3$ specifically focused at a laser excitation wavelength, 248 nm, previously demonstrated as slightly below the threshold for triple dissociation into H, CO and OCH_3. These measurements of the internal energy images of translational features and of FTIR probing of the vibrational and rotational energy deposited in two radical fragments from excited molecules without a sufficient energy for further decomposition, provide patterns of internal energy distributions and in particular of the roaming phenomenon. By extensive simulations, we had indications of a quasi-Boltzmann behavior of the rotational energy distribution of the CO product from the open channels. Such an assumption justifies the disentangling of signals from alternative paths to the detected products, enforcing the fitting of data as the sum of different populations with a Boltzmann profile. On the other hand, the sampling of initial conditions in classical molecular dynamics, indicates a role of conical intersections for populating high-lying regions of the ground state potential energy surface.

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8th photo dynamics

Relevance of Photophysics to the Measurement of the Electronic Spectra of Radicals and Ions

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A number of modern approaches of chemical physics and spectroscopy are used to identify for the first time the electronic spectra of reactive intermediates of organic molecules. The species investigated are intermediates in terrestrial processes such as combustion leading to the formation of aromatics, and in interstellar environments of diffuse and dark clouds and planetary nebula. In the laboratory the species are produced in situ within supersonic expansions using discharges and laser vaporization and detected in small concentrations by laser methods ranging from resonance enhanced multi-photon ionization, to cavity ring-down and degenerate four wave mixing [1]. The spectroscopic information within the electronic spectra, supported by theoretical calculations enables the structure of the species to be identified. The experimental knowledge of the electronic transitions also provides the means of in situ monitoring of such reactive intermediates in inaccessible environments.

The limitation of the approaches is dictated by the photophysics of the excited electronic states. The unpredictability of the excited state's photophysical behavour has implications for comparison with astronomical measurements [2]. Furthermore this can be exploited as a means of detecting the electronic transitions, as is demonstrated for mass-selected cations at 10 K in a radiofrequency trap, following collisional relaxation with cryogenically cooled helium gas [3]. Reversible photoinduced isomerizations of mass-selected protonated polycyclic aromatic hydrocarbons in 6 K neon matrices are observed by monitoring their electronic absorptions [4].

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Water through Graphynes' Pores: First Principles Penetration Barrier and Force Field Optimization

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Graphynes are novel twodimensional carbon-based materials, naturally presenting a nanoweb-like structure characterized by triangular and regularly distributed pores[1]. These intriguing features make them appealing for molecular filtering, especially for water purification technologies. First principles calculations are carried out at the MP2C level of theory to properly assess the interaction between water and graphyne, graphdiyne and graphtriyne pores. The computed penetration barriers suggest that water transport is unfeasible through graphyne while being unimpeded for graphtriyne. Nevertheless for graphdiyne, which presents a pore size almost matching that of water, a low barrier is found which in turn disappears if an active hydrogen bond with an additional water molecule on the opposite side of the opening is taken into account (see Figure). These results confirm the possibility of an efficient use of graphtriyne (and larger pore homologues) membranes for water filtration and purification, as very recently suggested by molecular dynamics investigations[25]. Still, in contrast with these studies[25], present findings do not exclude graphdiyne since the related first principles penetration barrier leads to water permeation probabilities[6] which are at least two orders of magnitude larger than those estimated by employing generic force fields[25]. The computed energy profiles for graphdiyne have also served to build a new pair potential for the water--carbon noncovalent component of the interaction which better represents the water--pore behaviour[6] and it is recommended for molecular dynamics simulations involving graphdiyne and water.

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Resonant Nature of the Raman Response and Solvent Effects in Molecule-Metal Oxide Nanoparticles Hybrids

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Surface Enhanced Raman Scattering (SERS) can be used as a probe of interfacial electron transfer, a critical process in solar cells, sensors, and photocatalytic systems. We discuss some recent results on assessing the influence of the solvent, as well as in clarifying some important issues about the resonant character of the Raman response of hybrids molecule/dye/semiconductor nanoparticles. Our results unequivocally indicate that in the presence of a solvent, there is a dramatic increase in the magnitude of the dynamic polarizabilities, which mirrors the experimental observations.

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Stochastic Dynamics of Two Level Systems: Langevin Canonical Approach

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A Langevin canonical framework for a two-level system coupled to a bath of independent harmonic oscillators was developed within a coupling scheme different from the well-known spin-boson model. Thermal equilibrium values were reached at asymptotic times by solving the corresponding set of nonlinear coupled equations in a Markovian regime [1,2]. In particular, values of both the population difference and coherences, phase difference thermal values (or, equivalently, the so-called coherence factor) and heat capacity through energy fluctuations were obtained and are discussed in terms of tunneling rates and asymmetries. The incoherent and coherent tunneling regimes are analyzed in terms of a critical temperature defined by the maximum of the heat capacity. The corresponding numerical results issued from solving a non-linear coupled system of equations are fitted to approximate path–integral analytical expressions [3] beyond the so-called non-interacting blip approximation in order to determine the different time scales governing both regimes.

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Excited state dynamics of metal and semiconductor nanoparticles

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This talk will describe theory work aimed at understanding the time evolution of metal (plasmonic) and semiconductor nanoparticles following ultrafast excitation, with emphasis on small particles (< 2 nm) where it is possible to describe the dynamics using quantum methods. In both cases the density of excited states is such that many electronic states are excited, and the initial dynamics (< 1 ps) is dominated by dephasing and electronic relaxation. On the 1 ps time scale, electron-phonon coupling is dominant, and then on the 100 ps time scale thermal energy in the nanoparticles flows to the surrounding medium. The theory methods use both time domain and frequency domain quantum descriptions for short times. Then on the ps and longer timescale we switch to continuum theory where the results depend on electron-phonon coupling strengths and on interfacial and bulk conductivities. If time permits we will describe our modelling of ultrafast experiments including TA and FSRS.

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Ultrafast Structural Deformation of Small Polyatomic Molecules by Coincidence Momentum Imaging and Laser Assisted Electron Diffraction

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It has been revealed from a series of our recent studies [1-3] that geometrical structure of molecules can be changed largely within a very short period of time when they are exposed to an intense laser field. Among such ultrafast processes, ultrafast hydrogen migration is noteworthy. We have shown that the migration of a hydrogen atom or a proton within a hydrocarbon molecule can proceed very rapidly within the duration of an ultrashort intense laser pulse. In order to probe these ultrafast hydrogen migration processes within CH_3OH in real time, we performed pump-probe coincidence momentum imaging measurements by using few-cycle laser pulses, and revealed that the hydrogen migration in the singly charged manifold, $CH_3OH^+ \rightarrow CH_2OH_2^+$, starts to proceed within the pump-probe delay time shorter than 20 fs. After introducing the recent experimental results, I will discuss possible mechanisms of this extremely fast hydrogen migration on the basis of theoretical wave packet simulations of the hydrogen migration on the potential energy surfaces of CH_3OH^+. For probing ultrafast structural deformation of molecules, we developed another technique called laser assisted electron diffraction (LAED) [4,5] by which ultrafast deformation of the geometrical structure of molecules can be probed in real time as a series of snapshots of electron diffraction patterns. The temporal resolution of this optical gating method can in principle be as short as the temporal duration of ultrashort laser pulses employed in the pump-probe measurements. On the basis of the LAED patterns of CCl_4 that we recently recorded, I will discuss possible future applications of this LAED method for determining instantaneous geometrical structures of polyatomic molecules.

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Modeling Photophysics in Organic Conjugated Molecules: Electronic and Vibrational Energy Redistribution

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In recent years we have witnessed rapid development of organic photovoltaic and light-emission research spanning multiple classes of small donor and acceptor conjugated molecules. Organic solar cells have great potential since organic materials have many advantages compared to traditional inorganic semiconductors.

In the present work, we investigate photoexcited dynamics and relaxation pathways in a variety of these molecules using Non-Adiabatic Excited State Molecular Dynamics (NA-ESMD) approach[1,2].

Firstly, we study the photodynamics of a spiro-linked conjugated polyfluorene that prevents π-stacking and, therefore, stabilizes the blue emission of polyfluorene films. This dimeric aggregate consists of two perpendicular α-polyfluorene chains that weakly interact between each other. After photoexcitation, an efficient ultrafast localization of all the electronic population in the lowest S_1 state is observed. Both, internal conversion between electronic excited states and electronic energy relaxation on one single electronic state contributes to this localization.

Secondly, we study the exciton (de)localization between two chromophore units in the weakly coupled anthracene dimer dithia-anthracenophane (DTA) during photodynamics. The initial excitation creates an exciton primarily localized on a single monomer unit. In the ensemble average, the localized initial exciton quickly delocalizes between both monomers within 10fs. However, our analysis indicates that delocalization within a single trajectory never occurs. In this sense, a collective delocalization phenomenon arises.

Finally, we analyze the photodynamics of several members of the family of cycloparaphenylenes (CPP), simple conjugated carbon nanorings consisting solely of benzene rings with para linkage. We discuss the evolution in time of the delocalization of the exciton among the different rings.

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Angular Distributions of Ionized Electrons Produced in Ion-Atom collisions

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The Fourier Transform applied to the Close-Coupling [1] amplitudes in the configuration space at the end of the collision, provides a continuous energy spectrum of electrons for the ionized electrons in ion-atom collisions.

In this presentation, the above procedure is exemplified in the proton-H and proton-He collisions at 50 keV impact energy. In the former case, the results are close to the experimental data between 10 and 30 eV. Above this energy range, the measurements go below our results. We believe this behavior in the cross section is due to contributions coming from low-energy ejected electrons, which were not included in absolute measurements. For the Helium target, the measurements were taken over a wide energy range, which after a comparison with our results, allow an estimate of the percentage with which the low-energy electrons contribute to the energy distribution for the H target case. As this approach gives reasonable electron energy spectrum for simple systems, its extension to more complex atoms seems adequate to understand higher complexity processes.

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8th photo dynamics

Why is the gas phase photoinduced isomerization of trans-Stilbene significantly slower than in the liquid phase?

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The photo-induced isomerization of trans-Stilbene has been studied with various means for over half a century. Yet even today, this benchmark system presents experimental and theoretical challenges. Perhaps the most profound of these is the measured slowing down of the room temperature isomerization rate in the gas phase (500-1000 psec) as compared to the rate in the presence of an unassociated liquid (30-100 psec).

Various reasons have been proposed to explain the measured slowing down. Schroeder and Troe and coworkers have suggested that the presence of a medium lowers the barrier height to isomerization. Leitner and Wolynes and coworkers have suggested that the medium increases the intramolecular vibrational relaxation rate of the molecule, thus increasing the isomerization rate. We have suggested that photo-excitation of the molecule creates a relatively cold nascent vibrational population which leads to a slow rate. The presence of a medium, causes reheating of the molecule and thus exponential increase of the isomerization rate.

In this talk we will present recent experimental measurements of the Ernsting group [1] which provide direct evidence that significant cooling of the molecule takes place upon excitation. These Femtosecond Stimulated Raman Scattering (FSRS) experiments provide a first direct observation of photoinduced vibrational cooling of Stilbene, yet they leave us with a number of non-trivial theoretical challenges.

Although the Stilbene system has for many years served as a prototype for the Kramers' description of chemical change, we will discuss why the Kramers' framework is not valid for this system. We will also note the conditions under which one should observe vibrational photoinduced molecular cooling. We will consider a theoretical framework for describing the FSRS experiments. Finally we will describe some of the remaining theoretical challenges and implications of the Stilbene system experiments on other photoinduced processes such as electron and proton transfer.

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Insights into Anionic States of Acetoacetic Acid from Photoelectron and Electron Energy-Loss Spectroscopies and Theory

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The anion photoelectron and electron energy-loss spectroscopies probe different regions of the anionic potential energy surface. The former probes the potential energy surface close to the minimum energy structure of the anion. The latter probes the anionic potential energy surface close to the minimum energy structure of the neutral. Both experimental techniques and theory have been engaged to study anionic states of acetoacetic acid (AA). The keto tautomer of AA, equipped with neighboring carboxylic and keto groups, is a promising system for studies of intramolecular proton transfer (*keto-ol*) driven by an excess electron. The anion photoelectron spectra are consistent with our theoretical prediction that the valence anion has the ol structure, i.e., the COOH proton is transferred to the keto group. However, the electron energy-loss spectra do not provide evidence for the ultrarapid proton transfer capable of competing with the spontaneous electron detachment. The computational results allow rationalizing these experimental findings in terms of the co-existence of various tautomers and conformers of the neutral AA. Only one, and not the most stable, keto conformer is prearranged for intramolecular proton transfer, and apparently it is not present in the gas of neutral AA with significant concentration. This conclusion is confirmed by vibrational spectrum of AA obtained in the electron energy-loss experiments: the carboxylic OH is not involved in intramolecular hydrogen bond, and thus the molecule is not prearranged for intramolecular proton transfer.

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Classical reactive scattering in a quantum spirit: Improving the shape of rotational state distributions for indirect reactions in the quantum regime

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For indirect triatomic chemical reactions under single-collision conditions, we propose a new implementation of the quasi-classical trajectory (QCT) approach to rotational-state distributions, of particular interest in the quantum regime where only a few rotational states are available to the products. This method is directly inspired from the amendments to be introduced in classical phase space theory (PST) in order to make it in exact agreement with quantum PST.

The approach is applied to the $D^+ + H_2$ and $H^+ + D_2$ reactions and the population of the rotational ground state is found to be in much closer agreement with the exact quantum one than the same population obtained by means of standard QCT calculations. The impact on the whole distribution is all the stronger as the number of available states is small. Lastly, the shape of the distribution appears to be controlled to a large extent by three factors, respectively called parity, edge and rotational shift factors [1].

Our method is a complementary alternative to the statistical QCT (SQCT [2-4]) method, often used to study indirect processes. However, contrary to what is done in the SQCT method, trajectories are not stopped at the entrance of the well(s) within our approach, thus expected to lead to reasonable predictions also for indirect processes that are not fully statistical, like those involving an osculating complex.

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8th photo dynamics

Studies of PCET in Natural and Artificial Photosynthesis

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Proton coupled electron transfer (PCET) plays a fundamental role in the mechanism of water-splitting at the oxygen-evolving complex (OEC) of photosystem II (PSII). We address the underlying reaction mechanism by structural studies of catalytic intermediates. Many physical techniques have provided important insights into the OEC structure and function, including X-ray diffraction (XRD) and extended X-ray absorption fine structure (EXAFS) spectroscopy as well as mass spectrometry (MS), electron paramagnetic resonance (EPR) spectroscopy, and Fourier transform infrared spectroscopy applied in conjunction with mutagenesis studies. However, experimental studies have yet to yield consensus as to the exact configuration of the catalytic metal cluster and its ligation scheme. Computational modeling studies, including density functional (DFT) theory combined with quantum mechanics/molecular mechanics (QM/MM) hybrid methods for explicitly including the influence of the surrounding protein, have proposed chemically satisfactory models of the fully ligated OEC within PSII that are maximally consistent with experimental results. The inorganic core of these models is similar to the crystallographic model upon which they were based, but comprises important modifications due to structural refinement, hydration, and proteinaceous ligation which improve agreement with a wide range of experimental data. The computational models are useful for rationalizing spectroscopic and crystallographic results and for building a complete structure-based mechanism of water-splitting assisted by PCET as described by the intermediate oxidation states of oxomanganese complexes. This talk summarizes recent advances on studies of the OEC of PSII and biomimetic oxomanganese complexes for artificial photosynthesis.

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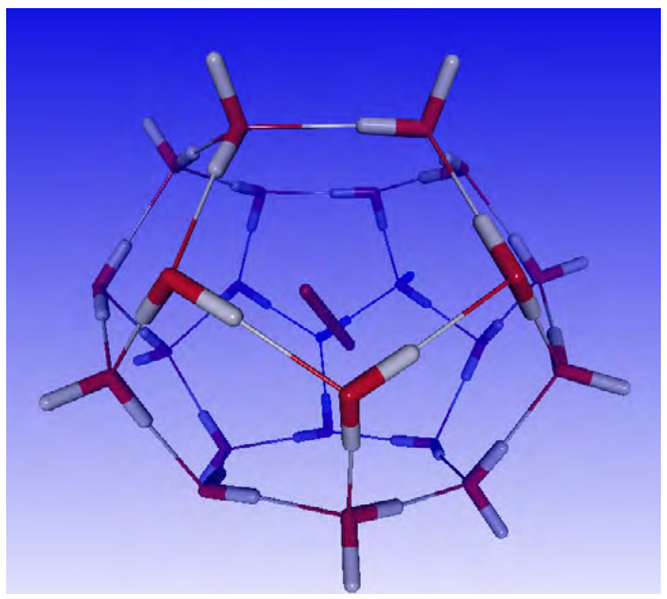

Local correlation studies of $Br_2(H_2O)_{N=4,5}$ clusters and $Br_2@5^{12}6^2$ clathrate cage

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The present work has been motivated by the wealth of detailed spectroscopic and dynamic information of bromine in clathrate cages generated by the groups of Janda and Apkarian [1]. These systems provide an ideal testing ground for theoretical studies of intermolecular forces and their effect on the spectroscopic properties of the guest molecule. For these many-body systems the use of standard ab initio methodology can become prohibitive and for this reason we have explored the use of density fitting(DF) and local correlation(LC) methods[2,3]. As a first test for this methodology we study the case of small clusters for which comparison with conventional methods is available [4]. We show that the DF-LC methods are able to reproduce the relevant structural and spectroscopic properties and have some advantages such as reducing the basis set superposition error which proves crucial for accurate estimates of the electronic shifts. However special care has to be taken with the different parameters involved particularly the Boughton-Pulay criterion which is critical for accurate results. The local methods allow an energy partitioning scheme [2] which is useful to gain insight into the main contributions to the interaction energy. We extend the studies to the case of $Br_2@5^{12}6^2$ exploring the energy dependence on the diatomic orientation finding the interaction is highly anisotropic and this reflects in the calculated electronic shifts. Using an angular distribution obtained from molecular dynamics simulations we make an estimate of the averaged electronic shift to be compared with experiment.

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Non-Markovian Optimal Quantum Control of Molecular Electronic States Employing Kadanoff-Baym Equations

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We propose a methodology to steer the ground state molecular orbital, to a predetermined CIS excited state, within vertical excitation approximation, employing optimal pulse-Shaping. The real-time propagation of the molecular orbital, takes into account electronic correlation and Non-Markovian effects, via the Green's function obtained by the self-consistent solution of the Dyson equation, within a second order approximation for the self-energy. We discuss and compare, the performance of the proposed methodology, computing the spectral function and its response to the optimal pulse-shape for a test bank, going from small to medium size molecules, employing for each one of them, a tailored even-tempered basis set as initial atomic orbitals.

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UV induced isomerization of deuterated Acetylacetone (D2) in Neon matrices

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Large amplitude intramolecular motions are generally coupled with other vibrational modes inside the molecule. One of the model system used to study this kind of process is Acetylacetone. A coupling between internal hydrogen transfer and methyl groups rotation was found in the chelated enol form [1]. Our goal is to elucidate the mechanism underlaying this process. On the other hand, previous studies in neon and para-hydrogen matrices showed the presence of two different groups of isomers after UV laser irradiation [2,3]. We chose an isotopologue of the original compound, in this case deuterated Acetylacetone (D2) in non-methyl hydrogens, in order to continue our studies with IR spectroscopy. We observed mainly the presence of the most stable isomer (chelated enol) after deposition in neon matrix, like in non deuterated Acetylacetone. Results also show the emergence of two groups of isomers after UV laser irradiation corresponding to non chelated enol forms. In contrast with normal Acetylacetone we were able to observe in each group a different population of isomers. In addition, we determined from the temporal behaviour of the sample (through IR spectra) the stability of isomers in each group, which agrees with theoretical calculations. IR laser irradiation of OD stretching overtones promoted isomerization process between isomers in the same group (OD rotation around CO bond), helping the assignments. These are the first steps in order to understand the photodynamics of this compound.

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Improvement of NIR Cyanine-Dyes Absorption Properties by Covalently-Bonded Auxiliary Chromophores

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We functionalized a cyanine fluorophore (emitter) widely used in microscopy with auxiliary chromophores (antennas). In these systems, the emission spectrum of the antenna section overlaps with higher electronic states of the emitter, which's fluorescence is induced indirectly by resonance energy transfer (RET) from the antenna sections. This design allows for modifications in the properties of the fragments separately and to add useful properties to the cyanine fluorophore, giving more degrees of freedom in the design of new luminescent markers. To verify that this design works, we synthesized two prototype molecules varying the antenna part: (a) using an anthracene derivative with a strong absorption in the UV range, and (b) using the well-known disperse orange 13 dye, which absorbs in the visible range and which can undergo photo-isomerization reactions [1]. Both antennas were linked to IR-780 cyanine, an infrared fluorescence emitter frequently used in microscopy [2]. We demonstrated that the antennas and the emitter act like independent chromophores, that they are coupled by RET and that the optical properties of the parent compounds can be used to predict those of the products. For the system with an anthracene derivative, the quenching of fluorescence of anthracene moiety and the excitation spectra of the cyanine fragment shows that RET occurs to the higher excited states of the cyanine. For the system that experiences photoisomerization, we demonstrated that the intramolecular RET can compete kinetically with the fast isomerization of the antenna, giving the cyanine a "photoswitch"-type behavior; this fluorophore design could be used in localization-based super-resolution microscopy techniques, where molecules that can switch between bright and dark emission states are required [3].

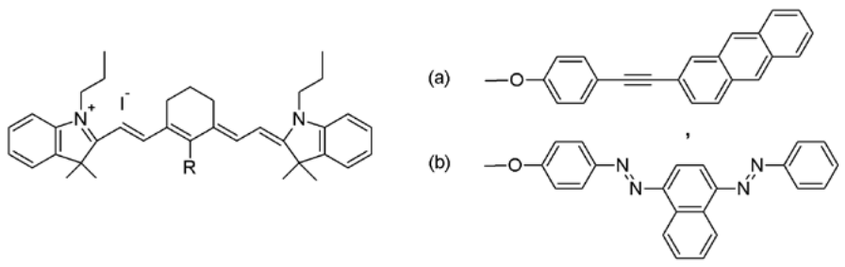

Figure 1. Synthesized prototype molecule.

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Electron propagator theory and its applications in molecular electronic structure

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Electron propagator theory provides a framework for the systematic inclusion of electron correlation in a one-electron picture of molecular electronics structure [1-3]. Instead of solving the many-body Schrödinger equation, sequences of propagators, also known as Green's functions, corresponding to a number of particles from one to the full, N-particle limit, are introduced to reformulate the many-body problem. Electron propagator theory provides a practical means of calculating electron binding energies, Dyson orbitals, and ground-state properties from first principles [3]. This approach to *ab-initio* electronic structure theory also facilitates the interpretation of its quantitative predictions in terms of concepts that closely resemble those of one-electron theories. In this work applications of electron propagator theory in the study of processes related to photo-ionization and their application in the understanding of the electronic structure of atoms and molecules will be discussed and explored.

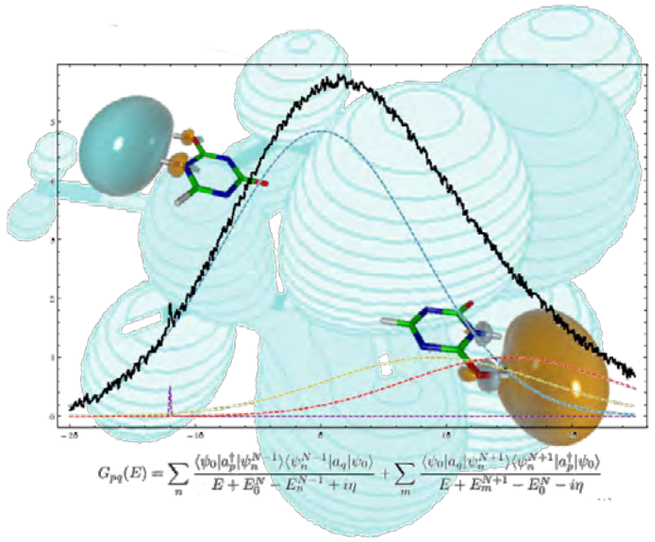

Figure 1. Dyson orbitals and photoelectron spectrum for 5-azauracil.

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8th photo dynamics

Influence of ultra-violet laser pulse on charge transfer and excitation processes in laser-assisted Li+ + H(1s) collision system

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The influence of an ultra-violet, intense (1.4 x 10^{13} W/cm^2) and ultra-fast (1 fs at FWHM) Gaussian laser pulse on the charge transfer and excitation processes for Li+ + H(1s), at 1-25 keV/amu impact energy collision range, is studied by direct numerical solution of the time-dependent Schroedinger equation. In order to model the structure electronic of the Lithium atom, we propose a pseudo-potential obtained within the Hartree-Fock approximation. Results of our numerical calculations are presented for the total, n = 2, and 3 charge transfer and n = 2 excitation cross-sections by projecting the stationary states of Lithium and Hydrogen neutral atoms to the total evolved wave function at the end of the collision dynamics, respectively. For the no laser case, we report a good agreement between our numerical results with available theoretical results [1,2] and experimental data [3] as reported in the literature, while the laser pulse improves the charge transfer process by a increment factor of 10 at 1-10 keV/amu .

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A Constrained-DFT Model for Photoinduced Charge-Transfer

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Among the many accessible sources of energy, solar energy is unique because it is available in sufficient amount in almost every part of the world. Solar energy research focuses on developing photosensitive compounds that mimic the process of solar energy absorption and conversion used by natural systems. Specifically, photoreceptive materials produce electron-hole (e^--h^+) pairs, which initiate the oxidation and reduction processes on adjacent substrates [1-2]. Accurate theoretical models of these systems can be used to guide the development of more efficient light-harvesting materials.

Density functional theory (DFT) is one of the most widely used approaches for calculating the electronic structure of molecules and materials. Local and semilocal functionals, like local density (LDA) and generalized-gradient (GGA) approximations, give reasonably accurate descriptions of ground-state properties. However, these functionals tend to dramatically underestimate band gaps and electron-transfer energies. A practical way around this problem is to use constrained density functional theory (CDFT)[3]. In CDFT methods, one minimizes the energy of a system subject to arbitrary constraints on the density. For example, CDFT allows us to exploit the accuracy of ground-state calculations to describe charge-transfer excited states. (Specifically, a charge-transfer excitation energy can be computed by taking the difference in energy between the ground-state and a CDFT calculation where the charge donor moiety is constrained to have one less electron, and the charge acceptor is constrained to have one more electron (relative to the ground state).) The aim of this work is to present a more robust CDFT method and show how it can be used to model electron transfer.

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8th photo dynamics

Experimental and Theoretical Study of the Modulation of the Intersystem Crossing in Aromatic Carbonyl Compounds

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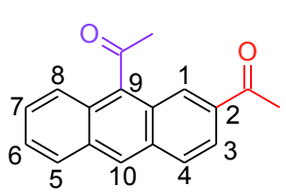
We investigated the photophysics of aromatic carbonyl compounds with the femtosecond fluorescence up-conversion technique. 9-acetylanthracene (9-AA) and 2-acetylanthracene (2AA) were chosen as models to study the modulation of the rate for Intersystem Crossing (ISC) in carbonyl compounds due to the presence and the relative energy of "receiver" states in the triplet manifold. Even though both molecules are isoelectronic and have the same carbonyl substituent, their photophysics are completely different.[1-3] It was found that for 9AA the time decays are in the picosecond regime: 0.6, 8 and 15 ps in cyclohexane, acetonitrile and methanol respectively. However, for 2AA, the decay times are of 0.8, 10 and 13 ns in the same solvents. The molecular geometries of the ground states were optimized using DFT and the excited state energies were calculated with the TD-DFT method, both at the PCM/PBE0/6-31G(d,p) level for the two compounds in the different solvents. The computational results correctly described the relative energy and the character of the S_1 and the first three triplet states of both molecules. It was found that the positions of the carbonyl substituent in 9AA and the interactions with the solvents induces a stabilization of a specific triplet state T_n with n-π^* character. This triplet (T_2) is close in energy to the S_1 state, thereby becoming a receiver triplet, and is responsible for the efficiency of the non-radiative channel (ISC). If the T_2 is not stabilized, the S_1 state will be deactivated via other channels (Fluorescence and Internal Conversion). In conclusion, the relative energy of a receptor triplet T_2 with respect to the S_1 state in carbonyl anthracenes strongly depends on the nature of the solvent and on the position of the acetyl substituent.



9AA and 2AA

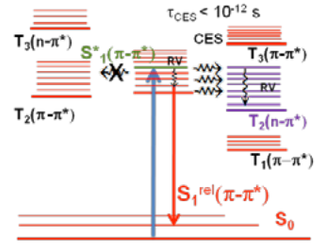


Figure 1. Scheme of ISC-fluorescence processes for the aromatic-carbonyl compounds (structure shown).

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Adsorption of Methyl Thiol on Silver Nanoclusters: Size Dependence

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Ligands with thiol groups have been widely used to protect noble metal nanoparticles, influencing their physical and chemical properties [1,2]. The adsorption energy of this kind of ligands on the metallic nanoparticle depends on the size and morphology, as well as the adsorption site on the nanoparticle (NP). The relevance of understanding the behavior of the adsorption energy respect to the NP size goes from the study of new catalysts [3] to self-assembly of complex structures [4].

In this work, we studied the adsorption energy and electronic structure of a single SCH_3 molecule on Ag_{13}, Ag_{55}, Ag_{147} and Ag_{309} NPs with icosahedral symmetry at different adsorption sites, letting a molecular dynamic procedure reach the most stable configuration through a code based on Density Functional Theory [5]. Three basic initial configurations were considered for the Ag-S bond: directly over an atom (top), between two (bridge) and three (hollow) silver atoms. The energies of similar adsorption sites of NPs with equivalent coordination numbers are compared. Furthermore, different orientations of the SCH_3 molecule were studied in search of a dependence of the adsorption energy. Adsorption on Nano clusters was compared to the adsorption on an infinite (111) silver surface taken as a limiting case of adsorption on large icosahedral clusters. After adsorption of the molecule, silver NPs exhibit a very small distortion in their atomic positions, evidencing that these high symmetry NP are stable under the process.

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Dynamics of the Formation of a Charge Transfer State and Symmetry Reduction in 1,2-Bis(9-anthryl)acetylene

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We studied 1,2-bis(9-anthryl)acetylene (BAAc) as a highly symmetric model compound for the characterization of the charge transfer process in an excited state involving a molecular symmetry reduction. Solvent polarity has a very important effect assisting the rearrangement of the electron density in the molecule. This system shows structural differences in comparison with the classic charge transfer model compound 9,9-bianthryl. [1-2] Due to the acetylenic bridge that joins the two anthracenic end-groups, BAAc minimizes steric hindrance between the end chromophores. The spectral evolution in acetonitrile and cyclohexane solutions were determined by femtosecond resolved up-conversion fluorescence measurements. The results show that for BAAc the formation of a charge transfer state occurs in two separate time scales initiated by the drastic polarizability increase upon electronic excitation.

The evolution of the emission spectrum involves a first reversible stage that occurs in 0.9 ps, where the fluorescence changes from a locally excited state (characteristic of non-polar solvents) to a partial charge transfer state. The second stage is the full charge transfer state formation that occurs in polar solvents on a time scale two order of magnitude longer.[3] Both steps are determined by the polarity of the solvent where the phenomenon takes place, stabilizing the changes in the electron distribution through the process.

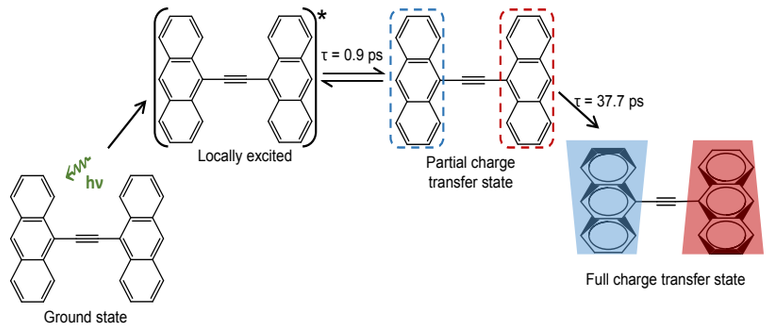

Figure 1. Steps for the charge transfer state formation in BAAc.

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Absorption spectral lines for water vapour at atmospheric temperature and pressure using a QCL and a power meter MCT

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The detection of atoms or molecules with high spectral resolution and high sensitivity has been a focus of attention in recent years, in fundamental spectroscopy, industrial[1], environmental monitoring[2] and recently medical applications[3]. The Quantum Cascade Laser (QCL) provides continuously tunable radiation in a wavelength range in the mid-infrared[4] (2-20 microns), which until recently was a region partially inaccessible. The availability of these lasers in this range, allows studies of vibrational transitions of molecules of interest in the above mentioned fields.

We present the results obtained in absorption spectroscopy, at atmospheric temperature and pressure, for several ro-vibrational transitions of water. These results were obtained using a nanosecond pulsed laser QCL, tunable in the range 6.71 to 8.73 micrometers. The absorption features were monitored using a power meter of the MCT type stabilized in temperature.

To obtain these results has been developed an automated data acquisition system in LabView. As the laser radiate in the spectral region where the normal vibrational modes of the molecule of water are located, the absorption spectra of this molecule is readily obtainable. This is in contrast to absorption spectroscopy in the visible and near infrared, in which the absorption process is induced by the excitation of vibrational overtones. The cross sections of the overtones are, in average hundreds or thousands of times smaller than the fundamental modes.

The spectral lines obtained with our experimental set up were compared with those reported in NIST, PNNL[5] and HITRAN, with satisfactory coincidences. This development opens the door to experiments with radicals in plasmas, which is the next step in our current research.

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Effect of the Relative Stability of the Triplet Manifold on the Photophysics of Nitrofluorenes

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Nitrated polycyclic aromatic hydrocarbon compounds (NPAH's) undergo ultrafast intersystem crossing (ISC) from the first singlet excited state S_1 (π–π^*) to a receiver triplet state T_n ($n \geq 2$) (n-π^*).[1] Nevertheless, the possibility has not been discarded that the ISC takes place between the S_1 directly to the T_1 state which may have a partial (n-π^*) character in some conformations. This idea has been tested by changing systematically the energy of the S_1 state so it can be located higher or lower in energy than the assumed receiver state T_n (higher-lying triplet). The Time-Dependent Density Functional Theory (TDDFT) allows to estimate the relative energies of the excited states of two analyzed molecules. The first one, 2-nitrofluorene (2-NF), shows the receptor T_n lower in energy than the S_1 state. The second molecule, 2-dietylamine-7-nitrofluorene (DEANF), maintains the receiver T_n higher in energy than the S_1. This is due to the fact that DEANF has a "push-pull" configuration which allows the aromatic system to stabilize the S_1 state.[2] The consequences of the change in the order of the S_1 and T_n states can be seen in the emission properties. 2-NF shows no emission spectrum and has a fluorescence quantum yield of $\Phi < 10^{-4}$. On the other hand, DEANF has $\Phi = 0.025$ in cyclohexane and shows double peaked fluorescence in polar solvents due to the formation of charge transfer states. The fluorescence life time (τ) of the S_1 state was determined with femtosecond fluorescent up-conversion techniques. For 2-NF $\tau < 200$ fs. This indicates that there is a highly efficient non-radiative process, such as ISC, deactivating the S_1 state. For DEANF $\tau = 100 \pm 4$ ps in cyclohexane, which shows that the process of deactivation of the S_1 state is much slower and allows competition between deactivation channels. The consistency of the TDDFT results with those of up-conversion allows to conclude that there is the need of the energetic coincidence between the S_1 and the T_n for an ultrafast ISC to take place. [3]

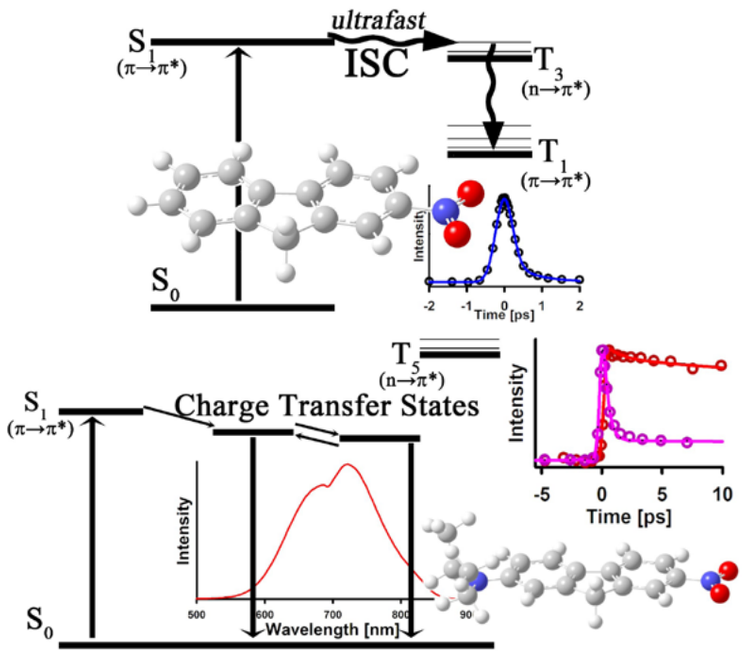

Figure 1. 2-NF (left) shows and ultrafast ISC and DEANF (right) shows formation of charge transfer states.

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Incoherent Broad-Band Cavity-Enhanced Absorption Spectroscopy for Trace Measurement of NO_2

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In the past decade, due to a growing awareness of the importance of air quality and air pollution control, many diagnostic tools and techniques have been developed to detect and quantify the concentration of pollutants such as NO_x, SO_x , CO, and CO_2. We present here the design and construction of an Incoherent Broad-Band Cavity-Enhanced Spectroscopy (IBB-CEAS) set-up which uses a LED emitting around 643 nm for the detection of NO_2. The LED light transmitted through a high-finesse optical cavity filled with a gas sample is detected by a low resolution spectrometer. This compact and inexpensive instrument is a promising tool for monitoring air quality among many other applications including the generation of traces in plasmas and molecular biological processes, among other uses.

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Application of an Optical Parametric Oscillator for Infrared Spectroscopy of Jet-Cooled Molecules and Complexes

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Van der Waals interactions are fundamental for molecular reactions such as aerosol formation, adsorption of atoms and molecules on surfaces, protein conformation and many more. Infrared absorption spectra of weakly-bound van der Waals complexes provide the necessary information to develop inter-molecular potential energy surfaces. During the past five years, our group has been systematically investigating the infrared spectra of weakly bound dimers and larger clusters formed from CO_2, N_2O, OCS, CS_2 and C_2H_2. The goal is to collect spectroscopic data against which theory can be benchmarked.

In 2013 our group developed and implemented a state of the art Optical Parametric Oscillator (OPO) based spectrometer for studying these intermolecular forces. The work presented will aim to explain the implementation of this OPO system and the process through which data is acquired. The main parts of the system, such as the cluster formation, probe laser and data processing, will be explained. Lastly some of the results will be shown demonstrating the efficacy of this method and the reliability of our setup as source for high-resolution and high-sensitivity spectroscopy of van der Waals molecular complexes.

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Contribution of the first hydration layer to the observed shift on the Br_2 absorption spectra on liquid water

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Since their discovery, solutions containing halogens like bromine or iodine have intrigued scientists due to the large shifts observed in their absorption spectra. Experimental results have shown halogen molecules are quite sensitive to the surrounding environment [1]. This feature has motivated several studies aimed to understand the role intermolecular forces between halogens and solvent molecules play on the absorption spectra, particularly on the different shifts observed in aqueous condensed phases, *i.e.* liquid water and ice solutions and clathrates [2].

In this work we look into the effect water molecules located on the first hydration shell of Br_2 have on the shifts of its electronic spectra. For this, we have analyzed several structures coming from a trajectory obtained from a Semi-Empirical Born Oppenheimer Molecular Dynamics (SEBOMD) study using an *ad-hoc* model for treating the Br_2-H_2O interaction, PM3-PIF. This semi-empirical model corrects the original PM3 description of the halogen-bond and the hydrogen bond [3]. EOM-CCSD calculations were done on systems containing Br_2 and a varying number of the closest water molecules, those placed at a distance smaller than the maximum of the peak corresponding to the first hydration shell in the radial distribution function, to evaluate their contribution to the shift observed in liquid water. (see Figure 1).

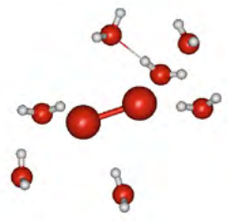

Figure 1 Snapshot of Br_2 with the closest water molecules in liquid water.

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Effect of Hg^{II} complexation on the spectroscopic properties of 8-HQ

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It is well known that very serious diseases are linked to the ingestion of heavy metals. In particular, the presence of Hg(II) has raised a lot of concern due to its accumulation in the food chain [1]. Ion-selective sensors represent a crucial part of the design of tools for qualitative and quantitative monitoring of metal ions in biological and environmental processes. The change of properties occurring upon the selective complexation motivates the development of specific sensor compounds. In particular, fluorescent chemosensors have become an interesting option [2] since it has been found that some ions lead to the enhancement of the fluorescence and some turn it off [3]. Aimed to understand the molecular basis of this behavior, in this work we present a study of the effect Hg (II) has on the spectra of 8-HQ (8-Hydroxyquinoline). For this, the structure of complexes of 1:1 and 1:2 stoichiometries were optimized at the MP2/6-31G(d,p) level and their electronic excited states studied with TD-DFT, in particular the changes occurring in the HOMO ® LUMO. We also analyzed, the effect coordinated water molecules on the cation have on the electronic transitions.

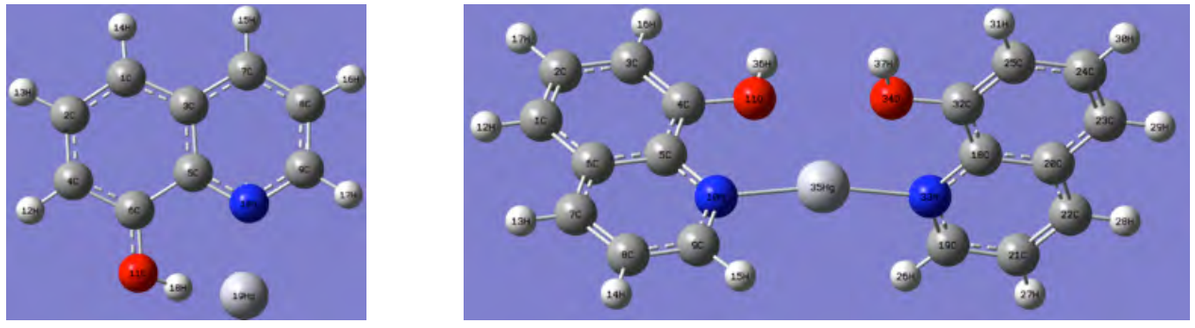

Figure 1. Structures of the 1:1 and 1:2 complexes of Hg (II) and 8-Hydroxyquinoline.

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Intermolecular forces in the 5^{12} cage of clathrate hydrates

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Interest in clathrate hydrates stems from both fascinating questions on their nature (intermolecular forces, spectroscopy and dynamics [1]) and also because of their relevance in applications ranging from natural gas reservoirs to hydrogen and carbon dioxide storage [2]. Their stability depends on the weak intermolecular forces between the guest molecules and a variety of polyhedral cages formed by hydrogen bonded water molecules. In this work we study the interaction of several guests with the smallest cage 5^{12}(dodecahedral) using *ab initio* methods. To analyze their stability we consider from the simple correlation with van der Waals radii to an energy partitioning scheme available for local correlation methods [3]. We also compare with a previous molecular mechanics study which proved successful in predicting clathrate stability [4].

We present a more detailed study for the case of chlorine where the question of its possible inclusion in the small cage has been the subject of debate from the original work of Pauling [5] who did not consider it possible until the recent X-ray study by the group of Ripmeester [6] showing occupancy. In this case the presence of halogen bonding depending on the model used to represent the cage is further analyzed.

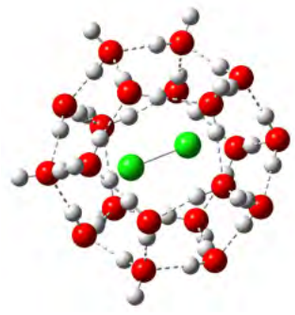

Figure 1. Cl_2 inside the 5^{12} cage .

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Understanding the ε→ζ phase transition of solid oxygen. Periodic HF and Density Functional Theory studies with localized atomic basis

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The ε and ζ phases of solid oxygen at pressures from 10 to 150 GPa are studied by periodic Hartree-Fock (HF) and DFT using different types of exchange-correlation functionals with gaussian atomic basis sets. Full geometry optimizations including atomic positions and unit cell parameters for the monoclinic C2/m structures were done. Vibrational calculations were performed at each pressure. Periodic HF does not predict the ε - ζ phase transition. While LDA and GGA Kohn-Sham methods predict too low transition pressures, the hybrid B3LYP approach accurately predicts the structural and electronic changes associated with the ε-ζ phase transition at 95 GPa. The evolution of the optimized B3LYP lattice parameters as well as the vibron frequencies *vs*. pressure are found in very good agreement with XRD experiments. We show that the greater stability of the ζ phase at higher pressures is critically due to the phononic vibrational contributions at finite temperature. The 1.3mH Gibbs free energy difference is in line with the coexistence of both phases in the 95-110 GPa range. The better agreement with experimental data at higher pressures is explained with CASSCF(8,8) as due to the increasing monoreferential character of the unit cell wavefunction. The mechanism for the non-conducting to the conducting phase at 100 GPa is explained via the electron pair localization function, where large opposite-spin electron pairing in the inter-cell regions of the ζ phase appears in the **ab** crystal planes.

Beam Propagation for Strain Measurement

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Optical methods are used as an alternative way to determine stresses, residual stress and deformation. For invasive tests the most used array is Moiré Interferometer doing the hole-drilling which provides a sensitive technique for measuring small surfaces displacements that occur in the experimentation [1]. There are also non-invasive optical methods, such as the Electronic Speckle Pattern Interferometer (ESPI) which is used with Moiré techniques [2]; another one extends conventional Moiré interferometry method to the micron-level spatial domain called micro-moiré interferometer [3].

The aim of the present work is to use one beam and study its propagation during a compression test, simulating a common column which is compressed by the whole building.

The simplest beam and the most known is the Gaussian type beam, as its characteristics and evolution are predictable [4]. Gaussian beams are able to pass through different media; in this case, the beam strikes a reflective spherical surface, it is taken as a mirror with a finite radii and it is known that is similar to a focal lens because the relation they have $f=R/2$. There are placed standardized probes of 1018 steel in the tension machine where compression tests are done [5]. A 1 mW laser is irradiating in the middle of the probe, it is placed a screen in order to record the reflected beam in a high resolution video camera. Once it is recorded the video of the reflected light, it is necessary to divide it into thousands of photograms in order to load each image and process it. A code is programmed in Matlab® for Digital Image Processing.

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Optical times response of an electrochromic device based on poly 3-hexylthiophene

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We prepared a simple electrochromic device based on the principle of electrolytic cell for studying oxidation-reduction response time of a semiconducting polymer, the poly 3-hexylthiophene (P3HT). The device was irradiated at a wavelength of 532 nm corresponding to polymer highest energy absorption; a voltage range was applied from 0V to ±1.5V because with higher voltage there is no change in the absorption spectrum.

The interest generated by this type of polymers (polythiophenes) is due to its molecular nature and possessing electron π delocalized that can be easily polarized in presence of an electric field [1], in addition to other properties such as its versatility in synthesis, thermal stability and processability [2]. Some of its derivatives have attracted attention because their high mobility of charge carriers in field effect transistors, as well as in manufacture of photovoltaic diodes for solar cells. From the results obtained show that the optical response is more noticeable for negative voltages (reverse polarity) Figure 1; the sample absorption intensity with and without voltage remained constant at least for 2 minutes that was the time relaxation.

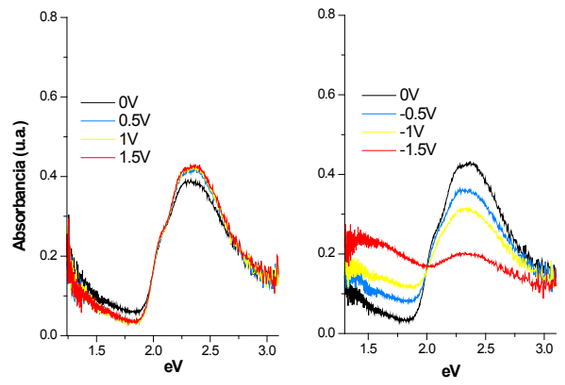

Figure 1. Absorption spectrum of electrochromic device-P3HT for different voltages.

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Aligning VP6 nanotubes detected by laser

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In this present work we used a kerr cell to align and even oscillate biological nanostructured materials; alignment has a great importance to futures application in electronics, optoelectronics, materials and even medicine. It is well known that the biological structures are highly selective and specific for its own construction; nanotubes from viral proteins have been studied extensively especially came from rotavirus [1].

Experimental Procedure

A Kerr cell were used to induce a current in a sample of VP6 nanotubes functionalized with gold to align in a specific direction, a laser beam of 632.8 nm passes through the sample to detect the phenomenon.

Results

It was found that the VP6 nanotubes were aligned and due to external applied electric field, these structures undergoing structural torque and it causes oscillation.

Conclusions

It is possible oscillate nanostructured materials with the application of an external electric field and depending on the field strength, these structures could align or oscillate.

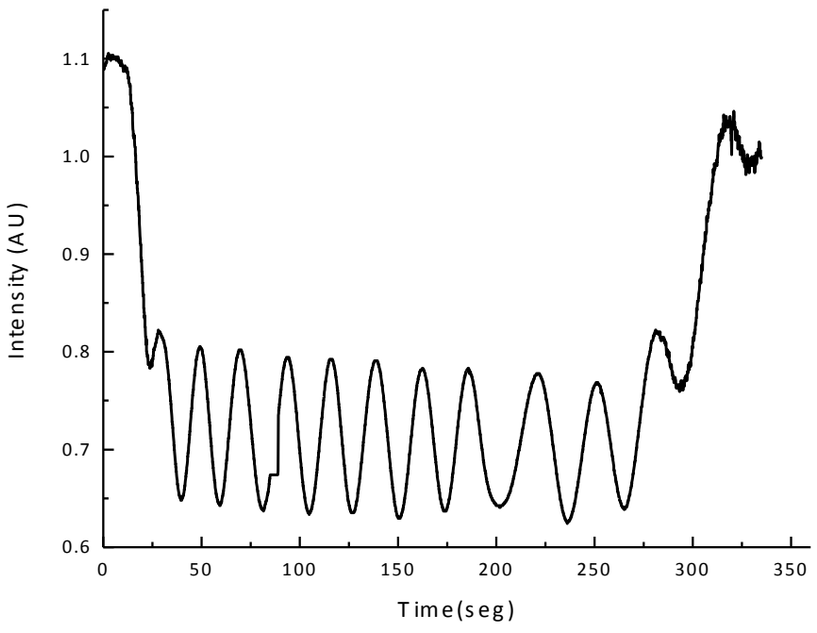

Figure 1. Intensity versus time of VP6 nanotubes under an electric field.

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Comparing Cl and CN Hydrogen-Abstraction Reaction Mechanisms in Gas and Liquid Phases

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Sunlight-driven production of Cl atoms in the atmosphere initiates hydrogen abstraction from both biogenic and anthropogenic hydrocarbons. Reactions between Cl and the small alkenes we study form HCl through two mechanisms: direct abstraction and addition of Cl to the double bond followed by HCl elimination. We interrogate these reaction dynamics using velocity-map ion imaging in the gas phase, ultrafast vibrational probing in the liquid phase, and direct-dynamics simulations. The HCl from the direct mechanism appears with high kinetic energy, low rotational energy, and in nearly all energetically allowed vibrational levels. The indirect reaction mechanism, driven by large-amplitude motions of the Cl within the chloroalkyl addition complexes, is reminiscent of unimolecular roaming reactions and produces HCl with a characteristic rotationally hot distribution. Extending these experiments to H abstraction by photolytically produced CN radicals increases the complexity of the chemistry. Our suite of quantum-state resolved experiments on increasingly complicated systems provides detailed views of photoinduced bimolecular reactions that are important in both the gas and liquid phases.

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Photoionization and Excitation Mechanisms of Fullerenes and Hydrocarbons after Femtosecond Laser Pulse Irradiation

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Fullerenes are good model systems to study the excitation and ionisation mechanisms of complex molecules. Femtosecond photoelectron spectroscopy of fullerenes, like C_{60} and C_{70}, revealed highly excited Rydberg-like states.[1] The photoelectron spectra (PES) showed a thermal electron background and a peak structure superimposed on it below kinetic energies corresponding to the photon energy.[1] The peak structure could be assigned to one-photon ionisation of diffuse low-angular momenta states, so-called superatom molecular orbitals (SAMOs) centered on the hollow fullerene core, based on photoelectron angular distributions (PADs) and TD-DFT calculations.[1] Further studies on the fullerene species C_{82} and $Sc_3N@C_{80}$ showed PES and PAD with similar features.[2] The peaks become less prominent compared to the thermal electron background for increasing molecular size and decreasing symmetry and are almost absent for the endohedral species.[2] Therefore the thermal electron emission seems to be the main ionization mechanism for larger and more complex molecules at these excitation conditions.[2] The relative photoionisation probabilities of the s-SAMO to p- SAMO were analyzed for photon energies from 2-3.5 eV and showed good agreement with theoretical calculations.[3]

Quantum mechanical studies on a series of polycyclic aromatic hydrocarbons (PAH) revealed similar Rydberg-like molecular orbitals in analogy to the SAMOs in fullerenes and will be discussed. The binding energies of the s-state and the p_z-state show a decreasing trend with increasing molecular size.

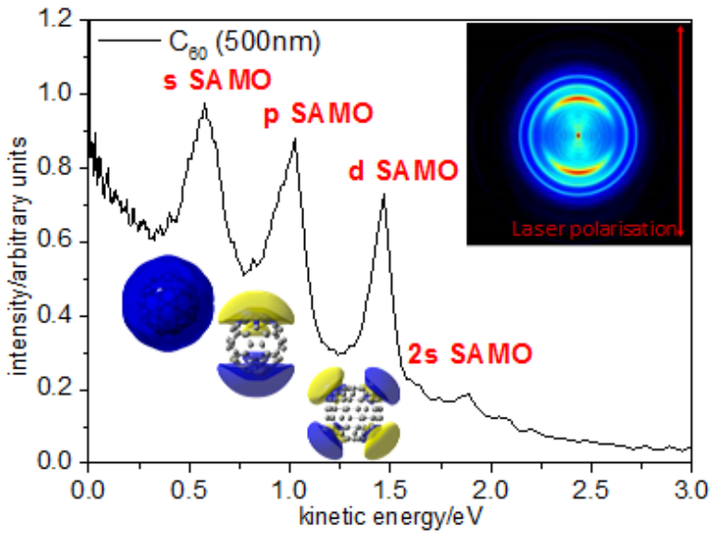

Figure 1. Angular-integrated photoelectron spectrum of C_{60} at 500nm with assignment of the peaks to the corresponding state and the theoretically modelled molecular orbital using DFT. On the top right the corresponding inverted VMI image is shown with the laser polarization along the red arrow.

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Acoustic waves from mechanical impulses due to fluorescence resonant energy transfer

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We present a momentum transfer mechanism mediated by electromagnetic fields that originates in a system of two nearby molecules: one excited (donor *D**) and the other in ground state (acceptor A). An intermolecular force related to fluorescence resonant energy or Förster transfer (FRET) arises in the unstable *D*A* molecular system [1,2], which differs from the equilibrium van der Waals interaction. Due to the its finite lifetime, a mechanical impulse is imparted to the relative motion in the system. We analyze the FRET impulse when the molecules are embedded in free space and find that its magnitude can be much greater that the single recoil photon momentum, getting comparable with the thermal momentum (Maxwell-Boltzmann distribution) at room temperature. In addition, we propose that this FRET impulse can be exploited in the generation of acoustic waves inside a film containing layers of donor and acceptor molecules, when a pico-second laser pulse excites the donors. This acoustic transient is distinguishable from that produced by thermal stress due to laser absorption (conventional photo-acoustic effect). The effect can be seen as exciting a vibrating system like a string or organ pipe with light. The FRET sound therefore provides a donor-acceptor specific opto-mechanical transducer that may enlarge the current capabilities of photoacoustic spectroscopy.

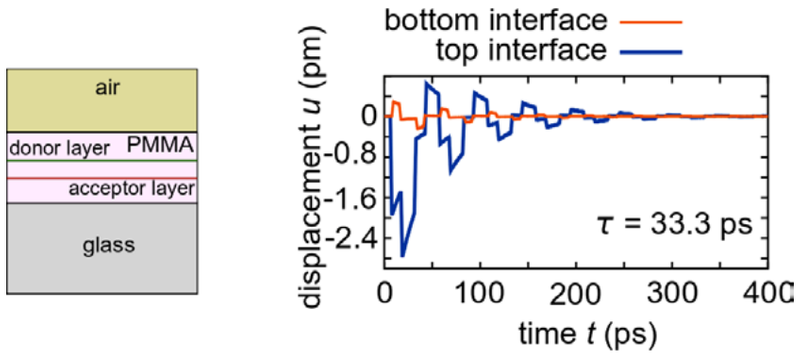

Figure1. Left: a PPMA film (20 nm thickness) with donor and acceptor layers. Right: dynamics of the displacement of PMMA-air/glass interfaces due to FRET impulse; τ is the *D*A* lifetime. See [3] for more details.

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Structural, thermal and magnetic properties of small nickel clusters

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In the last two decades nickel clusters have received considerable attention because of promising technological applications. As an example, the magnetic recording technologies require stable domains and a large amount of energy to produce magnetization reversal due to thermal excitations [1]. Magnetic properties of nickel clusters depend on its size and structure, and the identification of possible low energy structures are needed. In this work, ab initio calculations are performed to predict the minimal energy structures for Ni_n ($2 \leqslant n \leqslant 13$). The electronic structure has been computed in the DFT frame work using two different exchange and correlation functionals (PW91, PBE). An extensive total spin study and local minimum are presented Fig.1. The total magnetic moment is compared with previous experimental results [2], and free energy differences between some interesting clusters are sketched to propose possible mechanisms for transition between two close in energy structures.

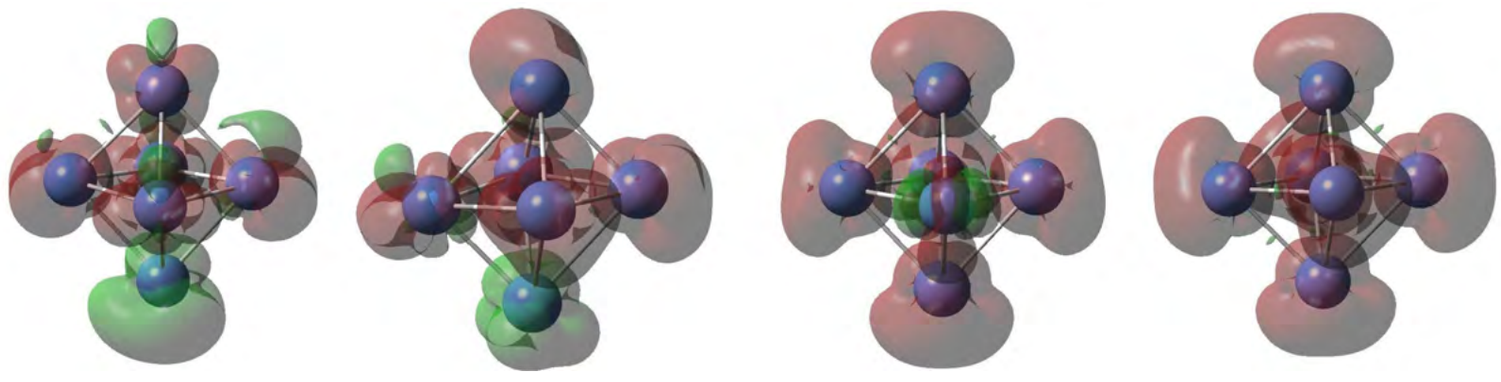

Figure 1. Spin densities for Ni_6

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SERS in Dopamine-TiO_2: influence of the chemical bond

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In this work we model the dopamine-TiO_2 interface on the atomic level using different approaches, in order to account for the Surface-enhanced Raman scattering observed in the system. These methodologies concern:

1) Periodic calculations using VASP for Dopamine on TiO_2 surfaces[1].
2) Molecular calculations for Dopamine-(TiO_2)n hybrids using Gaussian09, which gives non-resonant Raman spectra (no laser field nor excited states)[2].
3) Simplified model to probe SERS with stretched molecular geometries of Dopamine[3].
4) Development and implementation of a resonant Raman scattering activity equation. Transition dipole moments, oscillator strengths and excitation energies are obtained from TDDFT using G09.

We show that Dopamine molecule adsorbs dissociative in bidentate mode through O atoms on anatase surface for (001), (100) and (101) surfaces, decreasing the band gap of the system. In an eventual excitation a charge transfer is observed from molecule to the slab. Raman enhancement observed when Dopamine absorbs onTiO_2 clusters also involves normal modes related to a charge transfer. We show that the highest enhancement modes in the hybrid are present in stretched Dopamine. Concerning the Resonant Raman equation derived, we are currently comparing both resonant and non-resonant cases, as to explain why non-resonant Raman equations give quite accurate results for the resonant Raman response observed in experiments. To include relaxation processes and fluorescence, an analytical model is being developed using the Liouville equation/density matrix approach.

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A Classical Theory of Multichromophoric Resonance Energy Transfer

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Several energy transfer mechanism in photosynthetic light-harvesting systems predict a dramatic enhancement of the energy transfer rates [1–3], up to the order of interacting acceptors. Since the interactions between donors and acceptors induce delocalization of the excitation and at the same time may establish quantum correlations, this unexpected enhancement has been extensively related to quantum coherence between acceptors and donors.

However, the extend to which this enhancement is the result of purely quantum features and therefore, incapable of being present in a classical description of electronic energy transfer is not well stablished [3–5]. Based on previous works [6, 7] on the description of radiationless energy transfer in molecular systems using classical electrodynamics, we formulate a classical theory capable of predicting such enhancement.

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Structure and stability of C_7H_n molecular dications generated by X-rays photoionization of toluene

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The structure and stability of C_7H_n dications generated by X-rays photoionization experiments of toluene around the C1s edge is investigated through Density Functional calculations. The measurements were done using time-of-flight mass spectrometry, photoelectron-photoion coincidence techniques and synchrotron radiation. Around 70 initial geometries for each dication were optimized at the M06-2X/cc-pVTZ(-f) level of theory. Frequency calculations and thermochemical analysis were performed for the 15 most stable structures of each species. For the parent dication $C_7H_8^{2+}$, *ortho*- and *metha*-protonated benzyl cations are the most stable structures, highlighting the loss of structural integrity from neutral toluene and in conjunction with previous works [1]. Moreover, at this level of theory a previously non-reported methyl-biscyclopropenyl $C_7H_6^{2+}$ structure is 6.5 kcal mol^{-1} more stable than the cycloheptatrienylidene dication, usually assumed as the most representative structure of the system. For the $C_7H_4^{2+}$ species, a structure containing a planar tetravalent carbon (ptC) is energetically equivalent to the cyclic structure shown in Figure 1. Finally, the most stable structures of $C_7H_2^{2+}$ and $C_7H_3^{2+}$ present linear carbon arrangements, being 2.4 kcal mol^{-1} and 19.2 kcal mol^{-1} more stable than the less energetic cyclic structures, respectively.

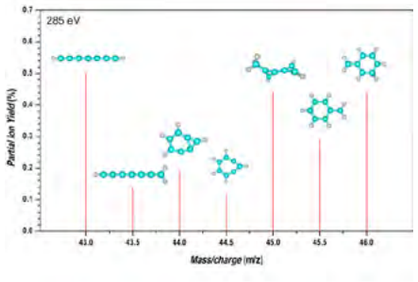

Figure 1. Partial ion yield (%) of dicationic products of toluene from X-rays photoionization experiments and their most stable structures at the M06-2X/cc-pVTZ(-f) level of theory.

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Fine and Hyperfine Structure Effects in Molecular Photoionization: a Model to describe Line Intensities

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Photoionization has recently become an increasingly widely used method to produce molecular ions in selected rovibronic quantum states for subsequent spectroscopic or collision experiments [1-3]. To interpret the results of such experiments, the populations of different fine- and hyperfine states in the molecular ions are important. Common models used to describe the relative intensities of different transitions in the photoionization process [4-5] do not provide information about the intensities of transitions between particular fine and hyperfine structure states of the neutral precursor molecule and the photoion, respectively, as these transitions are usually not resolved in photoionization spectra.

We are at the moment developing a theoretical model to describe the relative intensities of such transitions in the photoionization of diatomic molecules. Our model extends previous photoionization models [4-5] to include fine and hyperfine structure terms. It describes the intensities of such transitions in terms of angular momentum coupling coefficients and a few transition matrix elements, which can be obtained from *ab initio* calculations or treated as free parameters to be determined from experimental data. On our poster, the theoretical background of this model as well as results obtained so far will be shown.

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Ab initio Intermolecular Potentials of NO-H_2 in the ground and first Rydberg states

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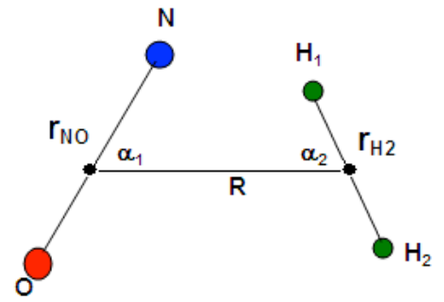
The motivation for this work comes from spectroscopical studies on the ultrafast structural response of solid parahydrogen upon photoexcitation of NO present as an impurity[1]. From previous studies on the related case of a neon matrix we know that a theoretical perspective based on a combination of ab initio interaction potentials and molecular dynamics simulations is useful to gain insight into the dynamics of the so called electronic bubble formation and decay[2]. In the case of parahydrogen the possible role of quantum delocalization and the limitations of a classical treatment suggest alternative methods based on quantum dynamics might be required[3].

In this work we present *ab initio* intermolecular potentials for the NO-H_2 system in the ground and first Rydberg state(A) involved in the electronic bubble formation. This is the first step towards a more comprehensive theoretical study of this problem. The intermolecular potentials are calculated in four dimensions keeping the intramolecular distances fixed(see figure). The level of theory is RCCSD(T)/AVTZ with additional diffuse s,p and d functions for NO and the 3s3p2d1f1g set of midbond functions. Symmetry allows us to treat the excited state as lowest for its symmetry for the present calculations but it is possible to extend the calculations to lower symmetry as has been discussed in our previous study of NeNO[4]. A comparison of the interaction potentials for ground and Rydberg state as well as their generalities will be discussed.



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8th photo dynamics

Electronic Structure and Spectroscopy of O_2 and O_2^+

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We carried out a comprehensive ab initio SCF MRD-CI study of the electronic structure of O_2 and O_2^+. Potential energy curves (PECs) of about 120 electronic states of O_2 and about 80 of O_2^+, as well as a number of states of O_2^{++} were computed. The cc-pVQZ basis set augmented with diffuse functions was employed. Spectroscopic parameters (T_e, T_v, ω_e, $\omega_e x_e$, B_e, D_e, D_0, μ, IP, etc.) are reported for several of the bound states and, generally speaking, a good agreement is found with the experimental counterparts. A preliminary sample of the results will be presented. The electronic absorption spectrum of O_2 has proved difficult to analyze/interpret due to the unusually large number of electronic states which arise from the peculiar open-shell structure of both the oxygen atomic fragments and the O_2 molecule. For instance, there are 62 valence molecular electronic states which correlate to the six lowest dissociation limits resulting from the three valence O-atom fragment states (^3P, ^1D, ^1S). In addition, there are several $nl\lambda$ Rydberg series converging to the $X^2\Pi_g$ ground ionic state and to the lowest two excited states $a^4\Pi_{ui}$ and $A^2\Pi_u$. Hence, the energy region below about 16 eV is rather congested with electronic states. Furthermore, a number of interactions of various types among them result in rovibronic perturbations which manifest themselves, e.g., as irregular vibronic structure, hence severely complicating the assignment of the absorption features and the analysis and interpretation of the spectrum. An overview of the electronic states and spectroscopy of O_2 will be presented. A chief motivation of this study of O_2 was to try to provide a theoretical insight on the nature, energetic position, shape, and dissociation asymptotes, of electronic states located in the 4 eV energy region encompassed between the O_2^+ ground state $X^2\Pi_g$ (IP=12.07 eV) and the first excited state $a^4\Pi_{ui}$ (IP=16.10 eV). This in order to aid in the interpretation of experimental data related to the mechanism(s) of the neutral dissociation of the O_2^{**} superexcited (Rydberg) states, which competes with autoionization. We are currently striving to compute PECs of relatively highly excited states of O_2 located in the 12-16 eV energy region which might help to visualize possible pathways for the neutral XUV photodissociation of the I, I' and I'' $^3\Pi_u$ superexcited states of O_2 leading to the $O(^3P)+O^*(^3S, ^5S)$ dissociation limits.

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Size Effects on the Thermal Performance Coatings Capturing Solar Energy

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In the present study the change in the internal heat generation was examined in thermal coatings by changing the composition of the system. The system consists of two layers, a layer of aluminum oxide supported on a porous crystalline aluminum substrate. The porous layer of aluminum oxide is exposed to radiation from sunlight and it is considered transparent, whereas crystalline aluminum layer is located behind it and it is considered opaque. The system has two layers of lengths L1 and L2 for the porous layer to the substrate which together have provided a total thickness of 0.4 mm. The heat transport in the bilayer system is described by the equation of energy conservation for each layer with a source term representing the absorption of radiation energy from the sun in the first layer, while the second equation layer presents no source term. [1,2] Boundary conditions arise from the temperature for the first layer as a boundary condition radiative rate, while the temperature at the opposite end of the system has a boundary condition convective type. [3] The system of equations is solved for steady state. Presented Graphs show the changes in temperature at both ends of the system and internal heat generation as a result of the variation in the thickness of the first layer in a range of 1 nm up to 1000 nm. Our most important result shows the asymptotic behavior in the internal heat generation beyond a thickness of 650 nm for the first layer. These results are of great interest in the design of coatings used in the industry for the photothermal solar energy.

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Importance of the electrolyte in the obtention of photoluminescent porous silicon: Optical and microstructural investigation

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In this work, we were obtained photoluminescent samples of porous silicon (PS) from (100) oriented n-type crystalline silicon. The porous silicon layers (PSL) were prepared by anodic etching with two different electrolytes, the first was composed by a mixture of hydrofluoric acid (HF) and ethanol (CH_3-CH_2-OH) in a ratio of 1:2, respectively. The second was composed by hydrofluoric acid (HF), ethanol (CH_3-CH_2-OH) and hydrogen peroxide (H_2O_2) in a ratio of 1:1:2 respectively. Raman scattering, photoluminescence (PL), gravimetry, scanning electron microscopy (SEM) and Energy Dispersive Spectrometer (EDS) measurements on the PSL were carried out. Raman scattering showed that the disorder in the samples obtained with hydrogen peroxide in the electrolyte is greater than in the samples obtained without this. The PL from PS increased in intensity with the increment in the anodization time and showed a blueshifted. the blueshifting of PL is consistent with quantum confinement of the electrons in the silicon nanocrystallites, the size of this nanocrystals was estimated in 3.08, 2.6 and 2.28 nm. The gravimetric analysis showed that the porosity increases with the incorporation of hydrogen peroxide in the electrolyte. SEM images showed an increment in the quantity and in the porous size, this is in agreement with the Raman results.

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Theoretical characterization of the optical activity of new coumarin-benzo-indolizine compounds

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Nonlinear optics is an important research field in photonics, where materials with optical activity can be used to manipulate optical signals.[1] The coumarins are molecules of interest due to its fluorescence, high quantum yield and photo-stability properties.[2] Moreover, the Indolizines have displayed interesting luminescence and pharmacological properties and they are easily functionalized to obtain derivatives as the pyrrole-pyridine-isoindol, with great light emission properties, Fig.1a), and used as materials to build optic sensors.[3] The properties of those molecules is a motivation for their synthesis with coumarin-benzo-indolizine nuclei, and theoretical-experimental characterization of their optical properties, in particular, self-phase modulation effect. In the present contribution we perform a theoretical characterization of molecules with coumarin-benzo-indolizine nuclei. The results show that the tertiary amine group is fundamental in the charge transfer process. In addition the analysis of the Molecular Orbitals (MO), Fig.1b), enables us to rationalize the excitation phenomena of the observed UV-Vis optical activity.

a) b)

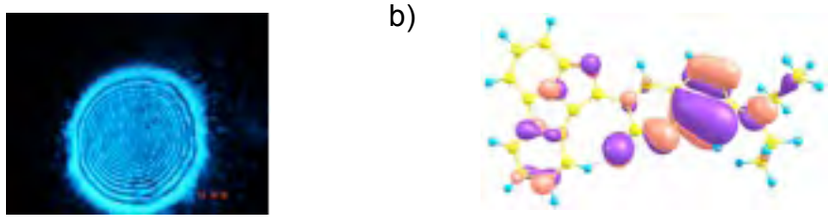

Figure 1. (a) Auto-diffraction rings of an organic molecule with non-linear optical behavior. (b) HOMO-3 of coumarin-benzo-indolizine derivative.

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Optical Sensor for the Determination of Chemical Species in Aqueous Media Based on the Excitation of WGM in Microcavities

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In this work, we develop an optical sensor for determining low concentrations of chemical species in aqueous media based on Whispering Gallery mode (WGM) microresonators. WGM microresonators were fabricated from fused silica, a material available and inexpensive. While cylindrical resonators were obtained by removing the primary coating to an optical fiber whose surface roughness is low enough for the development of sensors, microspherical resonators were produced by melting the tip of an unjacketed optical fiber, as molten fused silica takes a spheroidal shape due to surface tension. Quality factors were achieved in the range 10^5 in both cases, given the humidity of the environment to be submitted these sensors when considered in practical applications. Along with a reliable procedure for making tapered optical fibers to excite the WGM in the cavities, we show the potential of this technology to measure low concentrations (<1%), for which was taken as an example glucose solutions.

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DFT, Spectroscopic and Ultrafast Studies of triaryl and Tetraaryl Boron Compounds

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Arylboron componds in the singlet and triplet-states have been studied by means of femtosecond absorption pump-probe spectroscopy and fluorescence spectroscopy with picosecond time resolution. The transient species in microsecond time resolution were identified by flash photolysis technique. In the ground-state of trigonal molecules, the electron density is located in the phenyl groups and after excitation; the empty pz orbital is populated, delocalizing the electron density between phenyl and boron centers. Tetrahedral arylborates reveal within the framework of excitation coupling between phenyl subsystems where the coupling depends on the interatomic twist angle. The ultrafast pump-probe absorption spectra shows a TICT band at 650 nm for Bph_4 and $B(p\text{-toluyl})_4$ systems, which have similar spectra position of the TICT band of Biphenyl molecule. This last band is not observed for trigonal arylboranes, indicating an important participation of the geometric structure of arylboron compounds to possibility the electron delocalization between the rings. DFT studies of each boron system indicates a relevant delocalization of the π-orbitals around of rings in the singlet-state.

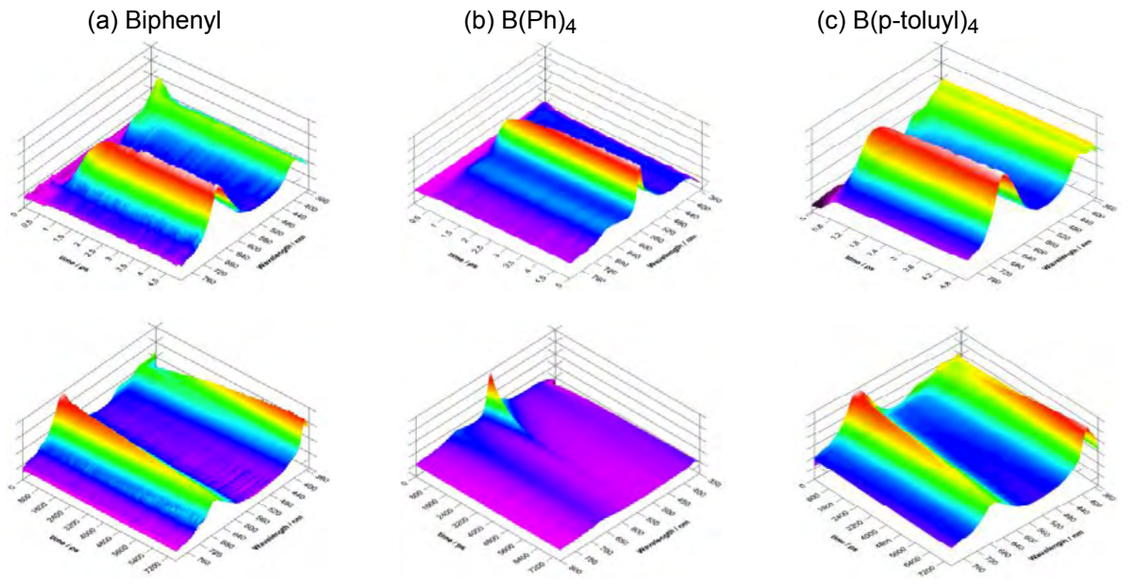

Figure. Ultrafst pump-probe 3D kinetic for (a) Biphenyl, (b) $B(Ph)_4$ tetraphenylborate and (c) $B(p\text{-toluyl})_4$ tetrap-toluylborate in short (above) and long (below) time-scales.

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Emission properties of interacting quantum dots embedded in a microcavity

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In this work, we consider a micropillar with a micracavity that has quantum dots embedded. These quantum dots can interact by Forster interaction. The main question that we solve is how the geometric distribution can affect the statistical properties of the light produced by the system. In particular, we found analytical expressions to determine when the system can present crossing or anticrossing relations in the band diagram allowing to optimize the intensity of the emission spectrum [13].

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Change of optical properties in ZnO nanoparticles doped with Mn, Cu and Ni and functionalized with organic acids

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ZnO nanoparticles are an attractive choice as host semiconductor due to its low toxicity, cost, stability and high transparency in the visible wavelength [1]. Doped nanomaterials have many interesting and unique properties that are useful for important technological applications [2,3]. Nowdays the use of nanocomposites in biosensing, through the use of their optical properties, is an increasing area in research. The surface coverage leads to electronic passivation, which enhances room temperature photoluminescence of the nanomaterial and could then be used as fluorescent probes for the study of biological samples. In doped ZnO nanostructures with transition metals have been observed a change in magnetic and optical properties respect to ZnO [4].

This study reports Mn, Cu and Ni doped ZnO nanoparticles surface modification using isonipecotic acid (IA) and 3-mercaptopropionic acid (AMP). The nanostructures were characterized by different spectroscopy and microscopy techniques. The measurements showed highly crystalline material with nanostructures size of about 3-4 nm. Their optical properties were also evaluated from solid UV-Vis and fluorescence techniques.

We obtained the gap energy of the nanoparticles from UV-Vis measurements. In the case of Cu and Mn doped nanoparticles the value of the gap is lower than the one in non-doped nanoparticles. This behavior was not observed in Ni doped nanoparticles, and was associated with the higher Ni concentration in ZnO nanoparticles.

Fluorescence results show a change in excitation and emisión wavelength, disappearing the fluorescence in the case of Mn doped nanoparticles.

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First Stages of Porous Materials Synthesis: Molecular Dynamics Simulations

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Synthesis of porous materials from natural sources have attracted considerable attention due to their potential as catalyst, pharmaceutical industry, as well as promising applications in separation and support of large molecules. In the zeolite synthesis are involved a great number of molecular species, such as surfactants, aluminium and silicon oxides and water [1,2]. The details of the synthesis processes are very difficult to elucidate using experimental methods. Therefore, the use of simulations can help to know about the mechanisms involved [3]. In this sense, we have done Molecular Dynamics simulations of the first stages of the synthesis processes of porous materials using as source of silicon and aluminum different zeolite fragments. Cubic boxes formed by random distributions of DETAB surfactant, fragments of the natural zeolite clinoptilolite (with a ratio Si/Al=10) and water molecules in different ratios were modeled using periodic boundary conditions, in NPT ensemble at temperature of 300 K and 408 K and pressure of 1 atm. At 22 ns the Si and Al fragments are arrange forming layers and porous where the Al are located in the pore walls. These new mesoporous materials could have promising applications as catalyst and reservoir of large molecules.

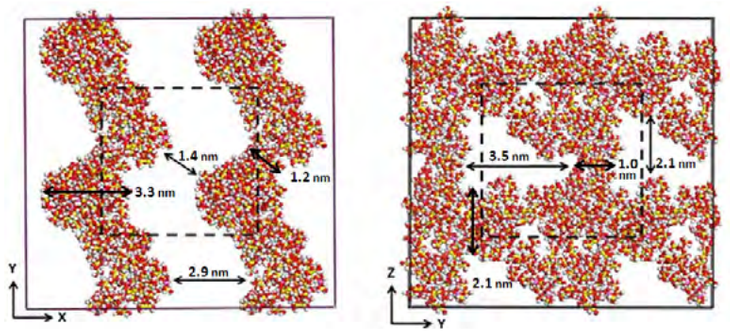

Figure 1. Different views of oligomers arrangement at the end of the simulation at 300 K

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Time-life calculations in self assembled quantum dots in the framework of k•p theory

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We present a theoretical study of life-time of excitons, in self-assembled InAs/GaAs quantum rings grown by droplet epitaxy. These nanostructures are shaped by two quantum dots, interacting by a quantum ring. Wave functions are calculated in the framework of the four-band **k•p** theory. Calculations include the strain potential and the gradient of indium concentration, which are important to get a realistic model of the nanostructure. Obtained wave functions, with and without indium gradient, are used to calculate the oscillator strength and the life-time of neutral excitons. Comparison shows that the gradient modifies the carrier states. Changes in life times are due to the new distribution of the charge inside quantum dots. We show that our experimental results and calculations are in good agreement. Finally, we find that exchange and Coulomb interactions have a weak influence in the energy of the carrier states.

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Theoretical tools for the computation of spectroscopic properties of transition metal complexes: the case of metallocenes

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Methods of density functional theory (DFT) offer important tools to predict features of vibrational and electronic spectra [1].

In this work, we introduce applications of DFT with a locally modified version of the Gaussian suite of programs [2] to calculate infrared spectra at harmonic and anharmonic levels and to define a first benchmark for metallocene derivatives (Fe, Ru, and Os) [3]. Relying on the experience acquired in similar studies on organic molecules [4], the following functionals were employed: BP86, B3PW91, B3LYP, PBE0 and CAM-B3LYP. The associated basis sets are LANL2DZ, Def2SVP, Def2TVPand a combination of Stuttgart relativistic small core pseudopotential and basis set on metal atoms with a 6-311G** basis set on the ligands. In the case of ferrocene, we also used a modified 6-31G* basis set (m6-31G*) on iron and either the 6-31G** or the SNSD basis set on other atoms.

Very good results are given by anharmonic calculations carried out using the B3PW91 functional [3], which could reproduce the entire spectrum of ferrocene; B3LYP confirmed to be the most suitable functional to reproduce vibrations of ligands, while PBE0 shown the best agreement with experiment, for what concern the metal-ligand vibrational frequencies.

Future works will be addressed to exploit time-dependent DFT methods, to determine features of electronic spectra of transition metal complexes.

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Molecular orientation: a prerequisite for enantioselective photodissociation processes

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The origin of chiral discrimination in nature is a fascinating topic that has not yet found unanimous consensus [1]. Among the candidates for processes that may originate chiral selection, we here discuss the interaction of matter with light.

Alignment and orientation of chiral molecules is crucial in the achievement of enantioselectivity in photodissociation processes [2]. Manifestation of chiral effects is well known in the case of photodissociation with circularly polarized lasers, *i. e.* in presence of a chiral source radiation, while is less evident when unpolarized or simply linearly polarized lasers are employed. Electrostatic hexapoles have been largely employed in the orientation of linear and symmetric-top molecules in supersonic beams. Recently, molecules of higher complexity, in specific supersonic beams of chiral (asymmetric-top) molecules, have been characterized and oriented for the preparation of experiments of photodissociation through non-circularly polarized light sources [3, 4, 5].

The correlation of vectors (velocity, transition dipole moment and electric dipole moment) in the dissociation of a prototypical chiral molecule, by a linearly polarized laser, shows how it leads to different angular distribution of photofragments for the two mirror forms of the chiral molecule and for the racemic mixture [6].

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Charge Transport in Single DNA Systems: Intermediate Tunneling-Hopping Regime

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The study of charge transport in DNA is crucial for the understanding of different biological processes as well as the design of future technologies based on devices at the molecular level [1,2]. At shorter distances, charge transport in single molecules is understood within the coherent tunneling framework where the conductance decays exponentially with length. While at longer distances, incoherent hopping dominates and conductance decreases linearly. Electron transport in DNA along the helix allows us to explore both regimes as well as the transition from one regime to the other. We present a series of theoretical studies, in collaboration with experiments, of charge transport in different DNA systems. We also explore an intermediate regime where coherent and incoherent transport can coexist based on a model first introduced by Büttiker [3] through his theory of partial coherent charge transport.

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Computational study of photoexcited dynamics in weakly interacting conjugated molecular aggregates

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Non-Adiabatic Excited State Molecular Dynamics (NA-ESMD) approach is applied to investigate photoexcited dynamics and relaxation pathways in a spiro-linked conjugated polyfluorene at room (T=300K) and low (T=10K) temperatures. This dimeric aggregate consists of two perpendicularly oriented weakly interacting α-polyfluorene oligomers. [1,2] The negligible coupling between the monomer chains results in an initial absorption band composed of equal contributions of the two lowest excited electronic states, each localized on one of the two chains. After photoexcitation, an efficient ultrafast localization of all the electronic population to the lowest excited state is observed on the timescale of about 100 fs. Both internal conversion between excited electronic states and vibronic energy relaxation on a single electronic state contribute to this process. Thus, photoexcited dynamics of the polyfluorene dimer follows two distinct pathways with substantial temperature dependence of their efficiency. One relaxation channel involves resonance electronic energy transfer between the monomer chains, whereas the second pathway concerns the relaxation of the electronic energy on the same chain that has been initially excited due to electron-phonon couplin. Our numerical simulations analyze the effects of molecular geometry distortion during the electronic energy redistribution and suggest spectroscopic signatures reflecting complex electron- vibrational dynamics.

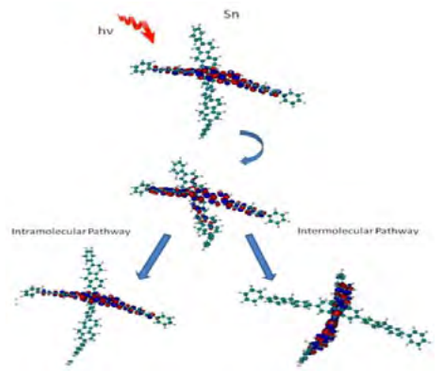

Figure 1: Energy transfer in spiro-linked conjugated polyfluorene.

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Representation of Potential Energy Surfaces of four-body systems by spherical coordinates: the case of CO - CO

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The use of spherical and hyperspherical coordinates, to represent potential energy surfaces, proved to be a useful tool for molecular dynamics simulations of systems involving four and five atoms [1].

The method relies on the expansion of spherical or hyperspherical harmonics of the interaction potential, which interpolates few significant points of the potential energy surface, called *leading configurations* (previously determined, for example by ab initio calculations or experimentally). It allows compactness and full account of the symmetry properties of the system. It is also important to highlight the following features: (i) the representation of the full potential energy surface can be improved simply by extending the set of leading configurations, or by replacing it with a more accurate one; (ii) the potential energy surface interpolates the points corresponding to the leading configurations; (iii) the analytical expression of the potential energy surface is suitable for structure and dynamical calculations [2-3].

Four-body systems that have been dealt with this method are O_2-O_2, N_2-N_2, N_2-O_2, H_2O – rare-gas-atom [3, 4] and CO – CO [5]

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Ab initio study of O_4H^+ : A tracer molecule in the interstellar medium?

George D. Xavier[1], Margarita I. Bernal-Uruchurtu[1] and Ramón Hernández-Lamoneda[1]
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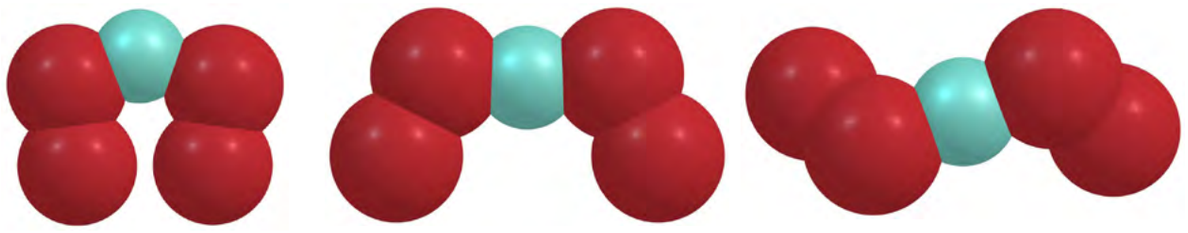
The structure and energetics of the protonated molecular oxygen dimer calculated via ab initio methods is reported. We find structures that share analogies with the eigen and zundel forms for the protonated water dimer although the symmetrical sharing of the proton is more prevalent. Analysis of different fragmentation channels at the CASSCF/ aug-cc-pVTZ level of theory show charge transfer processes which indicate the presence of conical intersections for various states including the ground state. An accurate estimate for the proton affinity of O_4 leads to a significantly larger value (5.2 eV) than for O_2 (4.4 eV), implying that the reaction $H_3^+ + O_4 \rightarrow O_4H^+ + H_2$ is exothermic by 18 Kcal/mol as opposed to the case of O_2 which is nearly thermoneutral. This opens up the possibility of using O_4H^+ as a tracer molecule for oxygen in the interstellar medium. More up-to-date calculations at the CI/aug-cc-pVTZ level of accuracy will also be reported.



(a) $^1A'$ (C_s) (b) $^1A_1$ (C_{2v}) (c) ^5A (C_2)

Figure 1 : Few minimized geometries of O_4H^+ at CASSCF level (a,b) and RCCSD(T) level (c)

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Oaxaca

Muy pocas partes en México poseen la riqueza y el patrimonio cultural que posee Oaxaca. La ciudad capital que lleva el mismo nombre, se considera como una zona propiamente turística, ya que ésta es la actividad de mayor importancia en la economía de la misma.

Dentro de la ciudad de Oaxaca se cuenta con uno de los patrimonios arquitectónicos más importantes y variados en el país, por lo que se recomienda recorrer y admirar la exuberancia de su barroco de escultura y pintura, retablos y yeserías de sus magníficos templos de los siglos XVI, XVII y XVIII, que junto a edificios neoclásicos y art-nouveau de la época independiente de México hacen a esta ciudad única; la gran variedad de museos como el Museo de las Culturas de Oaxaca, el Museo de Sitio Casa Juárez, el Museo de Arte Contemporáneo, el Museo Rufino Tamayo, el Museo del Palacio Espacio de la Diversidad (Palacio de Gobierno), el Museo Religioso de la Soledad, el Museo Textil de Oaxaca o el Museo de los Pintores de Oaxaca.

El arte se encuentra en cada rincón de Oaxaca y se puede admirar tanto en las diversas e interesantes galerías del Centro Histórico de la ciudad de Oaxaca, como en las maravillosas artesanías que reflejan el colorido y vivo espíritu de las diferentes regiones del estado como: piezas de barro negro de San Bartolo Coyotepec, cerámica vidriada de Atzompa, textiles de lana de Teotitlán del Valle y Santa Anta del Valle, alebrijes de San Martín Tilcajete o San Antonio Arrazola, cuchillería, trabajos de hojalata, magníficas piezas de la orfebrería y platería oaxaqueña, ropa típica, cestería, objetos de palma, talabartería, etc.

Oaxaca es famosa por su gastronomía, resultado de la fusión de las cocinas prehispánica y europea, siendo una de las más diversas y ricas del país. Tanto en la gran cantidad de restaurantes con los que cuenta Oaxaca, como en las famosas fondas de los mercados, se pueden degustar exquisitos platillos como los moles (negro, amarillo, verde, chichilo, coloradito, colorado o almendrado), el quesillo, los chapulines, el tasajo, la gran variedad de tamales, la cecina enchilada, las típicas nieves, las refrescantes aguas, las enormes tlayudas, los dulces regionales y bebidas ancestrales como el mezcal o el tejate.

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Atractivos turísticos

EL ZOCALO DE LA CIUDAD DE OAXACA

El zócalo de la Ciudad de Oaxaca o Plaza de la Constitución, centro de vida de la Verde Antequera, constituye el lugar por excelencia para empezar a disfrutar del ambiente y la hospitalidad oaxaqueña. Ha sido para la niñez de los oaxaqueños, de abuelos, de padres, de hijos y de nietos, un lugar de recreo, de emoción, de convivencia, de amor.

Todos los días es lugar de paseo, por su localización central, rodeada de los portales: Benito Juárez, de Claverías y de las Flores; así también por el Palacio de Gobierno (Portal de Mercaderes) y por la continuidad de espacio que da el atrio de la Catedral y la Alameda de León.

A su alrededor podemos disfrutar de excelente comida regional e internacional, así como la bebida de su preferencia, a su vez se ubican tiendas de conveniencia, tiendas de artículos fotográficos, etc. A sólo unos pasos se puede visitar la bellísima Catedral de Oaxaca, nuestros mercados donde se encuentran una gran variedad de artesanías, ropa típica, y los tradicionales puestos de nieve y dulces regionales. Pero especialmente, la Plaza de la Constitución es un lugar familiar y de esparcimiento sencillo y muy tradicional. Los niños encuentran en el zócalo un esplendido lugar para correr, perseguir a las palomas o disfrutar de una nieve.

Tomarse un café o una cerveza con cacahuates, escuchar a la banda de música, leer el periódico, ver pasar a la gente, escuchar la algarabía de los niños, el pregonar de los vendedores ambulantes o lustrarse los zapatos, forman parte de esta maravilla que solo Oaxaca puede ofrecer y que se ha perdido en el mundo.

El pueblo oaxaqueño tiene cuatro grandes pasiones: la música, la comida, la religión y la política. Todo esto podemos encontrarlo en la Plaza de la Constitución. Uno de los rasgos más sobresalientes del pueblo Oaxaqueño es la alegría de sus habitantes, hecho que se refleja en el colorido de sus tradiciones, los magnos olores de su gastronomía, la riqueza de sus celebraciones donde la música juega un papel protagónico, de gozo y celebración, de sonidos diversos que viajan en una atmósfera siempre de fiesta y en este lugar no podía faltar.

SERENATA DE LA MARIMBA DEL ESTADO

Por las noches, alternándose junto con la Banda de Música del Estado, en el zócalo de la ciudad de Oaxaca, los músicos que conforman la marimba del estado llenan de suaves sonidos el ambiente de este lugar con este instrumento de percusión compuesto de lengüetas de madera, parecido a un piano o a un xilófono, la música dulce de la marimba atrae a propios y a extraños. Ya sea un sabroso danzón o la trágica letra llena de amor y sentimiento de una canción de Chuy Rasgado, el sonido emanado de los golpes de las baquetas a la fina madera de la marimba parece llenar de alegría y emoción, los rincones del zócalo. Numerosos turistas y lugareños gustan de hacer una pausa en una esquina del zócalo para escuchar las armoniosas ejecuciones de expertos marimberos, y de repente se arma la fiesta y todo mundo se dispone a bailar en plena plaza principal, las sonrisas emergen espontáneas por doquier, todo por el hermoso sonido de la marimba.

CONCIERTOS DOMINICALES DE LA BANDA DE MUSICA DEL ESTADO DE OAXACA

La Banda de Música del Estado de Oaxaca ofrece conciertos dominicales también llamados "*Conciertos de Mediodía*" bajo un frondoso árbol de Laurel en el zócalo de la Ciudad de Oaxaca, justo enfrente del lado sur de la catedral de la Virgen de la Asunción. Para cerrar el concierto se toca la pieza "*Dios Nunca Muere*" de Macedonio Alcalá, una pieza himno para el pueblo oaxaqueño que vibra de emoción al escucharla.

La Banda de Música del Estado de Oaxaca ofrece un concierto que incluye música popular de varios ritmos así como piezas clásicas en el kiosco del zócalo de la ciudad de Oaxaca los días martes y jueves, así como los domingos debajo de uno de los impresionantes arboles de laurel que existen en este lugar. La gente se sienta a disfrutar hermosas melodías en las bancas que rodean al kiosco mientras degustan una rica nieve o bailan al son que la banda toca en las frescas tardes de la ciudad.

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MIERCOLES DE DANZÓN

Los miércoles en el Zócalo de la Verde Antequera, son de júbilo para los amantes del ritmo sabroso del Danzón. Los jóvenes de la tercera edad disfrutan enormemente cada semana de este ritmo cadencioso y propicio para el enamoramiento. Se puede apreciar la galanura de los bailarines, la elegancia de las damas que danzan suavemente al brazo de un experimentado y apuesto seductor. El envolvente ritmo del danzón, su rítmica elegancia, la precisión de los pasos, siempre exactos, sin apuro ni prisa, semilentos y provocativos, hacen de estas tardes momento propicio para dejarse llevar por la belleza de la música, su embrujo y su pasión.

La Plaza de la Constitución se viste de gala en verbenas populares, principalmente el 15 de septiembre Grito de la Independencia de México, el 23 de diciembre con la tradicional “Noche de Rábanos” y el 24 de diciembre con las calendas de Nochebuena, entre otras celebraciones importantes.

A unos cuantos pasos de la Plaza de la constitución y de la Alameda de León, podemos ubicar la calle Macedonio Alcalá, calle principal de Oaxaca, la cual es peatonal desde 1985. Conecta el Zócalo con el templo de Santo Domingo y se la conoce por Andador Turístico. Es el escenario del Museo de Arte Contemporáneo, de muchas casas coloniales antiguas, diversas galerías, restaurantes y las más distinguidas tiendas de joyas y artesanías. Al final de este Andador se levanta el excepcional templo de Santo Domingo, esplendor del barroco mexicano, con el altar mayor recubierto de hoja de oro, su impresionante decoración interior y el Museo de las Culturas de Oaxaca.

Disfrutar el zócalo de Oaxaca, la Alameda del General Antonio de León y todos los edificios que le rodean, así como la gente que se reúne, es un verdadero regalo que Oaxaca da generosa, a todo el público.

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UN POCO DE HISTORIA . . .

Esta plaza existe desde 1529, trazada por Juan Peláez de Berrio. Posteriormente, Alonso García Bravo la tomó como referencia o centro de la nueva traza urbana de la Villa de Antequera. Durante toda la epoca colonial, la Plaza no tuvo empedrado ni banquetas, sólo una fuente de mármol colocada en 1739. Dicha fuente fue quitada más tarde en 1857, para dar lugar a un primer kiosco rodeado de pequeñas arboledas. En el año 1881 se acordó una nueva compostura y ornamentación, excluyendo los árboles ya crecidos. El 15 de septiembre de 1885 se inauguró una estatua de Don Benito Juárez, colocada en el centro de la Plaza, una vez quitado el kiosco. Para 1901 volvió a ser reformado el sitio colocando el actual kiosco de influencia modernista o art nouveau. Su diseño refleja también el ambiente de la época porfiriana, por su estructura y cubierta metálica, así como por sus barandales de hierro forjado. En 1967 se adaptaron bajo el kiosco los servicios sanitarios y los locales comerciales; en el exterior se colocaron fuentes con figuras muy sugerentes, que más tarde fueron sustituidas por figuras caprichosas de cantera verde.

ANDADOR TURÍSTICO MACEDONIO ALCALÁ

A unos cuantos pasos de la Plaza de la constitución y de la Alameda de León, podemos ubicar la calle Macedonio Alcalá, calle principal de Oaxaca, la cual es peatonal desde 1985. Conecta el Zócalo con el templo de Santo Domingo y se la conoce por Andador Turístico. Es el escenario del Museo de Arte Contemporáneo, de muchas casas coloniales antiguas, diversas galerías, restaurantes y las más distinguidas tiendas de joyas y artesanías. Al final de este Andador se levanta el excepcional templo de Santo Domingo, esplendor del barroco mexicano, con el altar mayor recubierto de hoja de oro, su impresionante decoración interior y el Museo de las Culturas de Oaxaca.

Disfrutar el zócalo de Oaxaca, la Alameda del General Antonio de León y todos los edificios que le rodean, así como la gente que se reúne, es un verdadero regalo que Oaxaca da generosa, a todo el público.

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ZONA ARQUEOLÓICA DE MONTE ALBAN

En mixteco se conoce como Yucucuy, “Monte Verde” y en zapoteco es Daniva “Cerro Sagrado”, se cree que este sitio fue tanto habitacional como ceremonial.

Según Alfonso Caso, quien descubrió el magnífico tesoro de la Tumba No.7, en el siglo XVI estas tierras pertenecían a un soldado español de apellido Monte Albán o Montalbán, y es de donde se supone que viene el nombre de esta antigua ciudad.

Existen otras versiones a las que se les atribuye el nombre, por su similitud, el Monte Albano en Roma y por el árbol de casahuate que ahí florecía y cuyas flores blancas cubrían el monte.

Monte Albán se encuentra ubicado sobre tres cerros: Monte Albán, El Gallo y Bonete o Atzompa. Sus asentamientos más antiguos corresponden a la época I (500-100 a.C.). Fue durante esta época en la que se erigen gran cantidad de piedras grabadas conocidas como “Las Estelas de Monte Albán” o “Los Danzantes”.

Para la época II (100 a.C.200d.C.), Monte Albán tuvo un gran ascenso y se construyeron nuevas estructuras y se modificaron otras.

Monte Albán cuenta con una gran plaza que incluye varios edificios, entre los que destacan: el juego de pelota, el sistema M de los “Danzantes”, diversas tumbas siendo la más importante la número 7, la Plataforma Sur, la Plataforma Norte, así como el Patio Hundido.

El hallazgo más importante de este impresionante sitio, fue la Tumba No. 7, la cual después de ser abandonada (1300-1500 d.C.), fue reabierta por los mixtecos para enterrar a otros personajes importantes conservando los huesos y objetos de los señores zapotecos.

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En 1932, Alfonso Caso descubre en esta tumba uno de los tesoros más importantes de América Latina y el cual consistía en una rica ofrenda de más de 400 piezas de oro, plata, cobre, turquesa, alabastro, coral, hueso, perlas, conchas, cerámica, obsidiana, ámbar, jade, turquesa, cristal de roca, etc. Este magnífico tesoro se puede admirar en el Museo de Las Culturas del Centro Cultural Santo Domingo.

Últimamente se hicieron descubrimientos en la zona arqueológica de Atzompa, llegando a la conclusión de que este sitio era un barrio elite, que se construyó viendo a los palacios de Monte Albán y que había caminos y trazos visuales con vistas espectaculares. Desde ahí se veía la gran ciudad “sagrada”.

Asimismo, se encontró un horno de cerámica completo, lo que quiere decir que la tradición de hacer cerámica de esta comunidad, se remonta a la época de oro de Monte Albán.

Monte Albán se encuentra a 8 kilómetros de la ciudad de Oaxaca.

Links of interest:

http://www.oaxaca.travel/

http://www.visitMéxico.com/en/state-of-oaxaca

http://www.travelbyMéxico.com/oaxaca/

http://www.misiondelosangeles.com/

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Social program

Social and Cultural Activities
8 Photodynamics and Related Aspects Meeting

Hotel Misión de los Ángeles, Oaxaca
Octubre 26-31

Monday 27

10:00 – 13:00
Morning Walking Tour to the Historic Center of Oaxaca City
English speaking guide. Limited for 15 participants. FREE

18:00 – 19:00
Welcome mixer & A Mezcal tasting introduction

Tuesday 28

19:30 – 21:30 Patio Los Laureles
Science discussion cocktails and hors d'oeuvres

Wednesday 29

Excursion with english and spanish speaking guides.
Visit to Monte Albán Archaeological site and museum. 9 a 12hs
Visit to the Ex Convent of Cuilapam de Guerrero. 12:30 – 13:30
Lunch 13:30 – 15:00
Visit to the artisans in San Bartolo Coyotepec (Black pottery)
and/or San Andrés Tilcajete (Alebrijes) 15:30 – 16:30
Return to the hotel (17:30)

Interested participants must cover the excursion fee on Monday.
500 MXP for professors and 300 MXP for students and posdocs.

Banquet dinner 20:00 – 24:00
Served by Casa Oaxaca at the Patio of Palacio Municipal

Friday 31

Visit to Xoxocotlán's graveyard decorated for the All Saints' day and the day of the death festivities. (1 -2 nov) 19:00 hs.*

*This visit is OUT of the conference plan and only the transportation to and from the hotel will be organized.
Interested participants must reserve their place before Wednesday. 300 MXP.

Map

- Palacio Municipal / Banquet
- Hotel Misión de los Ángeles

TEMPLOS Y EX-CONVENTOS / CHURCHES AND EX-CONVENTS

1	Basílica de la Soledad	1-E
2	Carmen Alto	2-D
3	Carmen Bajo	2-E
4	Catedral	2-E
5	Ex-marquesado	1-D
6	El Patrocinio	2-D
7	Guadalupe	2-D
8	La Compañía de Jesús	2-E
9	La Defensa	2-E
10	La Merced	2-E
11	La Sangre de Cristo	2-E
12	La Santísima Trinidad	2-F
13	Las Nieves	2-E
14	Los Siete Principes	2-E
15	Nuestra Señora de Consolación	2-F
16	San Agustín	2-E
17	San Felipe Neri	2-E
18	San Francisco	2-E
19	San José	1-E
20	San Juan de Dios	2-E
21	San Matías Jalatlaco	3-D
22	Santo Domingo de Guzmán	2-E
23	Xochimilco	2-D

MUSEOS / MUSEUMS

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25	Belber Jiménez	2-E
26	Casa de la Ciudad	2-E
27	Casa Juárez	2-E
28	Centro Cultural Santo Domingo	2-D
29	Centro Fotográfico Álvarez Bravo	2-E
30	Fonoteca Eduardo Mata	2-E
31	Ex-Convento de San Pablo	2-E
32	Ferrocarril Mexicano del Sur	1-D
33	Filatelia (MUFI)	2-E
34	Instituto de Artes Gráficas de Oaxaca (IAGO)	2-D
35	Palacio Universum	2-E
36	de los Pintores Oaxaqueños	2-E
37	Religioso de la Soledad	1-E
38	Rufino Tamayo	2-E
39	Textil de Oaxaca (MTO)	2-E

LUGARES DE INTERES / PLACES OF INTEREST

40	Alameda de León	2-E
41	Arcos de Xochimilco	2-D
42	Casa de la Cultura	2-E
43	Cinema el Pochote	
44	Ex-convento de la Soledad	1-E
45	Ex-convento de Santa Catalina	2-E
46	Hemeroteca	2-E
47	Instituto Oaxaqueño de las Artesanías	2-D
48	Jardín Conzatti	2-D
49	Jardín el Pañuelito	2-E
50	Jardín Etnobotánico	2-D
51	Jardín Sócrates	1-E
52	Plazuela del Carmen Alto	2-D
53	Plazuela Labastida	2-E
54	Teatro Macedonio Alcalá	2-E
55	Universidad Benito Juárez	2-E
56	Zócalo	2-E

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57	Correos	2-E
58	Dirección General de Turismo Municipal	2-E
59	Instituto Nacional de Migración	2-E
60	Secretaría de Turismo	2-D
61	Telégrafos	2-E
62	Terminal de Autobuses de 1a. Clase	3-D
63	Terminal de Autobuses de 2a. Clase	1-E

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64	20 de Noviembre	2-E
65	Benito Juárez	2-E
66	De Abastos	1-E
67	De Artesanías	2-E
68	IV Centenario	1-E
69	La Merced	3-E
70	Sánchez Pacuas	2-D

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